```
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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  AUG 15  CAOLD to be discontinued on December 31, 2008
 NEWS  3  OCT 07  EPFULL enhanced with full implementation of EPC2000
 NEWS  4  OCT 07  Multiple databases enhanced for more flexible patent
                  number searching
 NEWS  5  OCT 22  Current-awareness alert (SDI) setup and editing
                  enhanced
 NEWS  6  OCT 22  WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                  Applications
 NEWS  7  OCT 24  CHEMLIST enhanced with intermediate list of
                  pre-registered REACH substances
 NEWS  8  NOV 21  CAS patent coverage to include exemplified prophetic
                  substances identified in English-, French-, German-,
                  and Japanese-language basic patents from 2004-present
 NEWS  9  NOV 26  MARPAT enhanced with FSORT command
 NEWS 10  NOV 26  MEDLINE year-end processing temporarily halts
                  availability of new fully-indexed citations
 NEWS 11  NOV 26  CHEMSAFE now available on STN Easy
 NEWS 12  NOV 26  Two new SET commands increase convenience of STN
                  searching
 NEWS 13  DEC 01  ChemPort single article sales feature unavailable
 NEWS 14  DEC 12  GBFULL now offers single source for full-text
                  coverage of complete UK patent families

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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FILE 'HOME' ENTERED AT 09:54:12 ON 16 DEC 2008
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=> file reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.21 | 0.21

FILE 'REGISTRY' ENTERED AT 09:54:22 ON 16 DEC 2008
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STRUCTURE FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0
DICTIONARY FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

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=> file caplus
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.46 | 0.67

FILE 'CAPLUS' ENTERED AT 09:54:37 ON 16 DEC 2008
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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s L1 SSS full
L1 NOT FOUND
The L-number entered has not been defined in this session, or it
has been deleted. To see the L-numbers currently defined in this
session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d his

     (FILE 'HOME' ENTERED AT 09:54:12 ON 16 DEC 2008)

     FILE 'REGISTRY' ENTERED AT 09:54:22 ON 16 DEC 2008

     FILE 'CAPLUS' ENTERED AT 09:54:37 ON 16 DEC 2008

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   0.48   1.15

FILE 'REGISTRY' ENTERED AT 09:54:52 ON 16 DEC 2008
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STRUCTURE FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0
DICTIONARY FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

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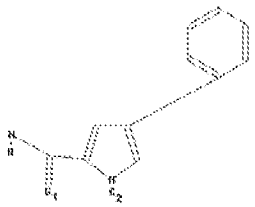
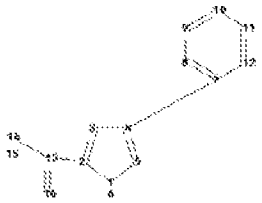
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

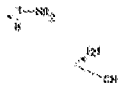
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

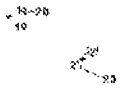
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10579825 H or CH3.str









chain nodes :
6 13 14 15 16 18 19 20 21 22 23
ring nodes :
1 2 3 4 5 7 8 9 10 11 12
chain bonds :
1-6 2-13 4-7 13-14 13-16 14-15 18-19 18-20 21-22 21-23
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-5 1-6 13-14 13-16
exact bonds :
2-3 2-13 3-4 4-5 4-7 14-15 18-19 18-20 21-22 21-23
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

G1:O,S,N,[*1],[*2]

G2:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d L1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> file caplus
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.46 | 1.61

FILE 'CAPLUS' ENTERED AT 09:55:11 ON 16 DEC 2008
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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

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http://www.cas.org/legal/infopolicy.html

=> s l1 SSS full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
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FULL SEARCH INITIATED 09:55:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11696 TO ITERATE

100.0% PROCESSED 11696 ITERATIONS 127 ANSWERS
SEARCH TIME: 00.00.01

L2 127 SEA SSS FUL L1

L3 43 L2

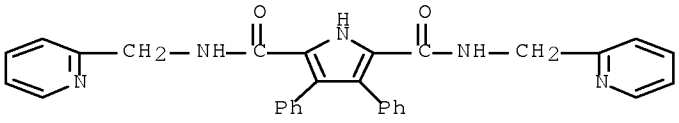
=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 43 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

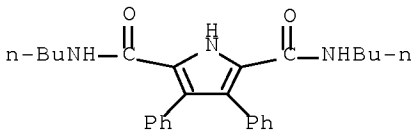
ACCESSION NUMBER: 2008:908277 CAPLUS Full-text
DOCUMENT NUMBER: 149:369113
TITLE: Structural diversity in the first metal complexes of 2,5-dicarboxamidopyrroles and 2,5-dicarbothioamidopyrroles
AUTHOR(S): Bates, Gareth W.; Gale, Philip A.; Light, Mark E.; Ogden, Mark I.; Warriner, Colin N.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Dalton Transactions (2008), (31), 4106-4112
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Metal complexes of 2,5-dicarboxamidopyrroles and 2,5-dicarbothioamidopyrroles were structurally characterized for the first time, complementing the significant amount of work that is reported for the analogous pyridine ligands. N,N'-Bis(3,5-dinitrophenyl)-3,4-diphenyl-1H- pyrrole-2,5-dicarboxamide forms octahedral bis(tridentate) complexes with Co(III) and Ni(II), where the ligands are bound to the metal centers through deprotonated pyrrole and amide N atoms. N,N'-Dibutyl-3,4-diphenyl-1H-pyrrole-2,5-dicarboxthioamide and N,N'-diphenyl-3,4-diphenyl-1H-pyrrole-2,5-dicarboxthioamide also form bis(tridentate) Co complexes, but are only deprotonated at the pyrrole N atom, the remainder of the coordination sphere comprising the thioamide S atoms. The di-Bu derivative was isolated as a Co(II) complex, whereas the di-Ph system deposited a Co(III) complex. In contrast, N,N'-dibutyl-3,4-dichloro-1H-pyrrole-2,5-dicarboxamide was found to act as a bidentate ligand in an octahedral Co(II) complex comprising two bidentate pyrrole ligands and two aqua ligands. Synthesis of N,N-bis(pyridin-2-ylmethyl)-3,4-diphenyl-1H-pyrrole-2,5-carboxamide gave a pyrrole ligand with increased denticity. Reaction with cobalt(II) chloride gave a dinuclear helicate complex. The ligand had undergone addition of a methoxy group to one of the linking methylene carbons, presumably as a result of the oxidative addition of solvent MeOH.

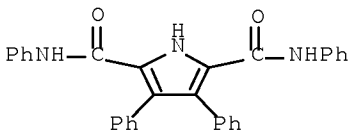
IT 1058152-04-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure; preparation of cobalt and nickel complexes of dicarboxamidopyrrole and dicarbothioamidopyrrole)
RN 1058152-04-7 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, 3,4-diphenyl-N2,N5-bis(2-pyridinylmethyl)- (CA INDEX NAME)



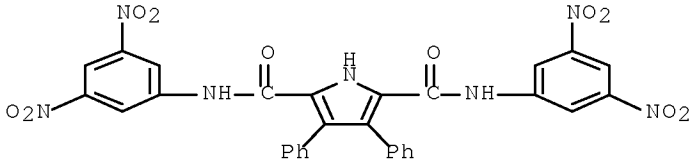
IT 365214-49-9 365214-50-2 566932-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cobalt and nickel complexes of dicarboxamidopyrrole and dicarbothioamidopyrrole)
RN 365214-49-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



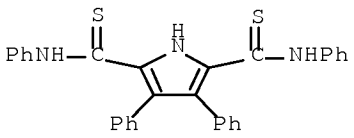
RN 365214-50-2 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



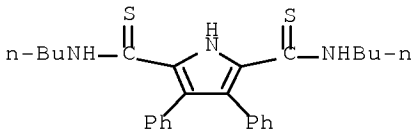
RN 566932-85-2 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(3,5-dinitrophenyl)-3,4-diphenyl- (CA INDEX NAME)



IT 1058151-99-7P 1058152-02-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cobalt and nickel complexes of dicarboxamidopyrrole and dicarbothioamidopyrrole)
RN 1058151-99-7 CAPLUS
CN 1H-Pyrrole-2,5-dicarbothioamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



RN 1058152-02-5 CAPLUS
CN 1H-Pyrrole-2,5-dicarbothioamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

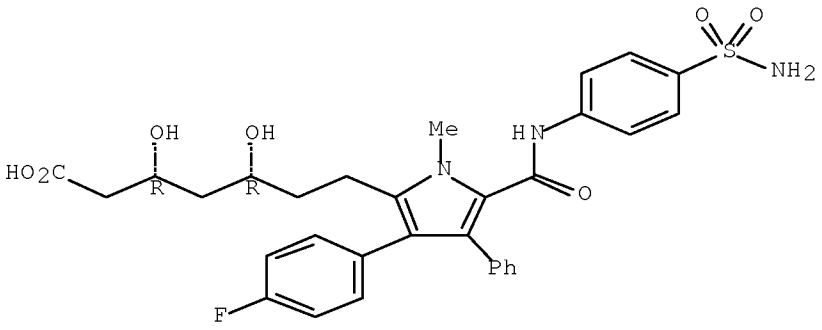
L3 ANSWER 2 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:696589 CAPLUS Full-text
DOCUMENT NUMBER: 149:143220
TITLE: Thermodynamic and Structure Guided Design of Statin Based Inhibitors of 3-Hydroxy-3-Methylglutaryl Coenzyme A Reductase
AUTHOR(S): Sarver, Ronald W.; Bills, Elizabeth; Bolton, Gary; Bratton, Larry D.; Caspers, Nicole L.; Dunbar, James B.; Harris, Melissa S.; Hutchings, Richard H.; Kennedy, Robert M.; Larsen, Scott D.; Pavlovsky, Alexander; Pfefferkorn, Jeffrey A.; Bainbridge, Graeme
CORPORATE SOURCE: Pfizer Global Research + Development, Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (2008), 51(13), 3804-3813
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Clin. studies have demonstrated that statins, 3-hydroxy-3-methylglutaryl CoA reductase (HMGR) inhibitors, are effective at lowering mortality levels associated with cardiovascular disease; however, 2-7% of patients may experience statin-induced myalgia that limits compliance with a treatment regimen. High resolution crystal structures, thermodn. binding parameters, and biochem. data were used to design statin inhibitors with improved HMGR affinity and therapeutic index relative to statin-induced myalgia. These studies facilitated the identification of imidazole 1 as a potent (IC50 = 7.9 nM) inhibitor with excellent hepatoselectivity (>1000-fold) and good in vivo efficacy. The binding of 1 to HMGR was enthalpically driven with a ΔH of -17.7 kcal/M. Addnl., a second novel series of bicyclic pyrrole-based inhibitors was identified that induced order in a protein flap of HMGR. Similar ordering was detected in a substrate complex, but has not been reported in previous statin inhibitor complexes with HMGR.

IT 1037300-11-0 1037300-16-5
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thermodn. and structure guided design of statin based inhibitors of HMGCoA reductase)

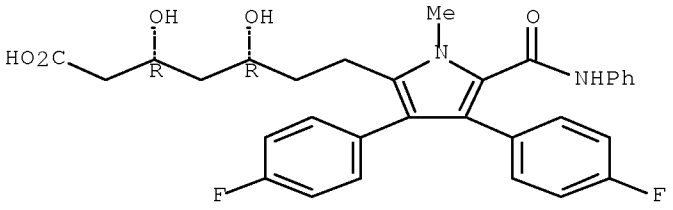
RN 1037300-11-0 CAPLUS
CN 1H-Pyrrole-2-heptanoic acid, 5-[[[4-(aminosulfonyl)phenyl]amino]carbonyl]-3-(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-4-phenyl-, (βR,δR)- (CA INDEX NAME)

Absolute stereochemistry.



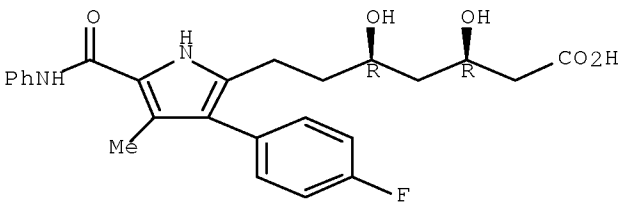
RN 1037300-16-5 CAPLUS
CN 1H-Pyrrole-2-heptanoic acid, 3,4-bis(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-5-[(phenylamino)carbonyl]-, (βR,δR)- (CA INDEX NAME)

Absolute stereochemistry.



IT 1037300-12-1 1037300-13-2 1037300-14-3
1037300-15-4 1037300-17-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thermodn. and structure guided design of statin based inhibitors of HMGCoA reductase)
RN 1037300-12-1 CAPLUS
CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)-β,δ-dihydroxy-4-methyl-5-[(phenylamino)carbonyl]-, (βR,δR)- (CA INDEX NAME)

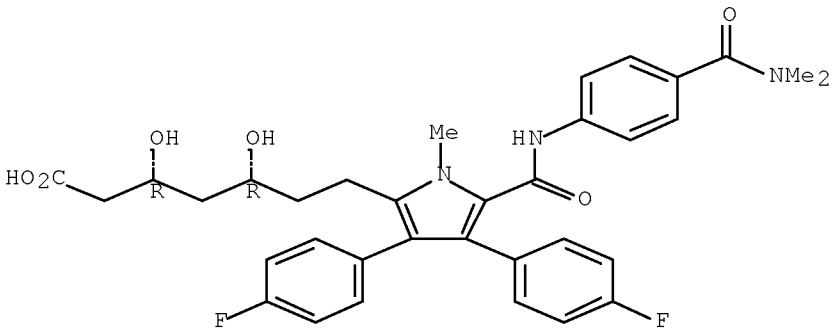
Absolute stereochemistry.



RN 1037300-13-2 CAPLUS
CN 1H-Pyrrole-2-heptanoic acid, 5-[[[4-

[(dimethylamino)carbonyl]phenyl]amino]carbonyl]-3,4-bis(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-, (βR,δR)- (CA INDEX NAME)

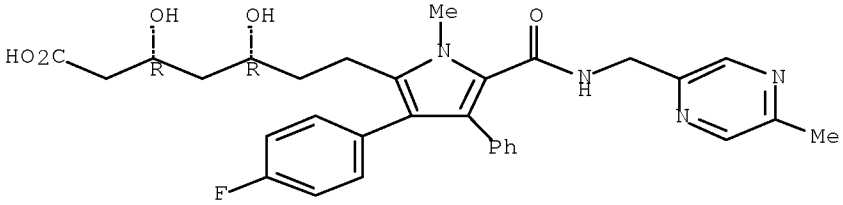
Absolute stereochemistry.



RN 1037300-14-3 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-5-[[[(5-methyl-2-pyrazinyl)methyl]amino]carbonyl]-4-phenyl-, (βR,δR)- (CA INDEX NAME)

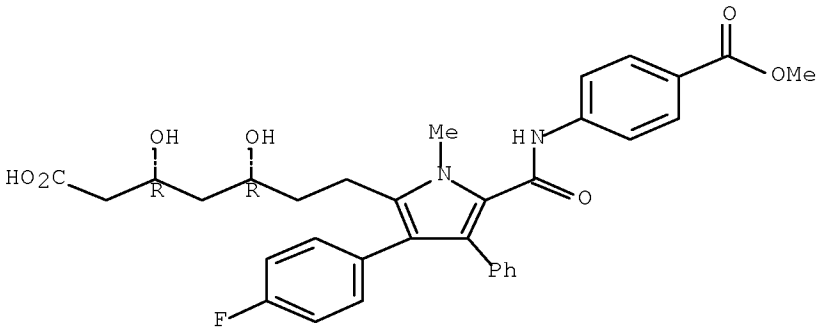
Absolute stereochemistry.



RN 1037300-15-4 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)-β,δ-dihydroxy-5-[[[4-(methoxycarbonyl)phenyl]amino]carbonyl]-1-methyl-4-phenyl-, (βR,δR)- (CA INDEX NAME)

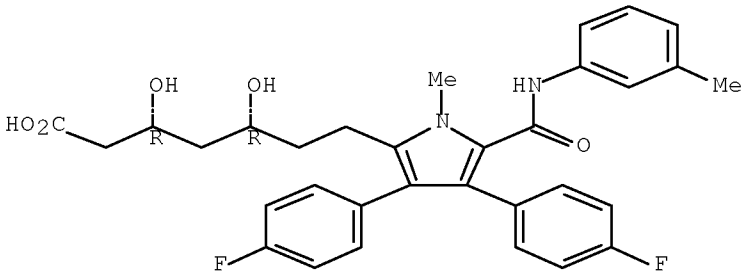
Absolute stereochemistry.



RN 1037300-17-6 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3,4-bis(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-5-[[(3-methylphenyl)amino]carbonyl]-, (βR,δR)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:43435 CAPLUS Full-text

DOCUMENT NUMBER: 148:144656

TITLE: Preparation of pyridinonyl PDK1 inhibitors

INVENTOR(S): Lind, Kenneth Egnard; Cao, Kathy; Lin, Edward Yin-Shiang; Nguyen, Thinh Ba; Tangonan, Bradley T.; Erlanson, Daniel A.; Guckian, Kevin; Simmons, Robert Lowell; Lee, Wen-Cherng; Sun, Lihong; Hansen, Stig; Pathan, Nuzhat; Zhang, Lei

PATENT ASSIGNEE(S): Sunesis Pharmaceuticals, USA; Biogen Idec, Inc.

SOURCE: PCT Int. Appl., 311pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008005457	A2	20080110	WO 2007-US15397	20070702
WO 2008005457	A3	20080724		

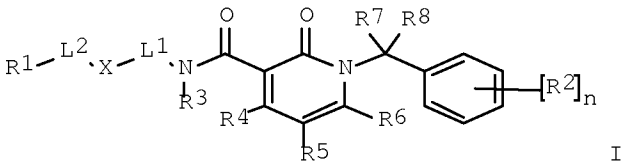
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2006-806414P P 20060630
US 2007-919057P P 20070319

OTHER SOURCE(S): MARPAT 148:144656

GI



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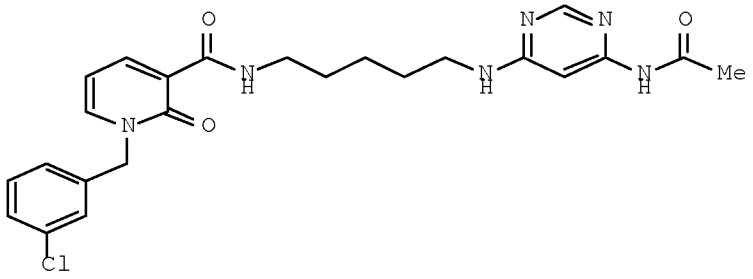


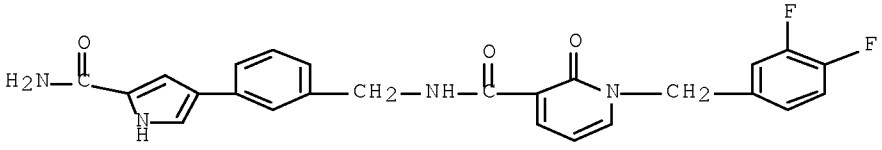
II

AB The title compds. I [n = 1-5; L1, L2 = a bond, O, NH, S, S(O), S(O)2, (hetero)alkylene; X = a bond, (hetero)cycloalkylene, (hetero)arylene; R1 = (hetero)cycloalkyl, (hetero)aryl; R2, R4-R8 = H, halo, OH, CF3, etc.; R3 = H, OH, CF3, alkyl, etc.], useful as 3-phosphoinositide-dependent protein kinase-1 (PDK1) inhibitors for treating cancer, were prepared E.g., a 2-step synthesis of II, starting from tert-Bu (5-aminopentyl)carbamate and 1-(3-chlorobenzyl)-2-oxo-1,2-dihydropyridine-3-carboxylic acid, was given. Exemplified compds. I were tested for PDK1 inhibitory activity in various assays (data given). Pharmaceutical composition comprising the compound I is disclosed.

IT 1001408-83-8P 1001408-97-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridinonyl PDK1 inhibitors for treating cancer)

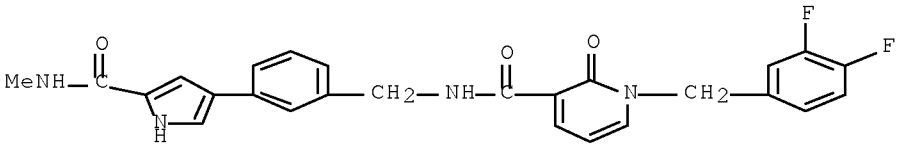
RN 1001408-83-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[5-(aminocarbonyl)-1H-pyrrol-3-yl]phenyl]methyl]-1-[(3,4-difluorophenyl)methyl]-1,2-dihydro-2-oxo- (CA INDEX NAME)



RN 1001408-97-4 CAPLUS

CN 3-Pyridinecarboxamide, 1-[(3,4-difluorophenyl)methyl]-1,2-dihydro-N-[[3-[5-[(methylamino)carbonyl]-1H-pyrrol-3-yl]phenyl]methyl]-2-oxo- (CA INDEX NAME)

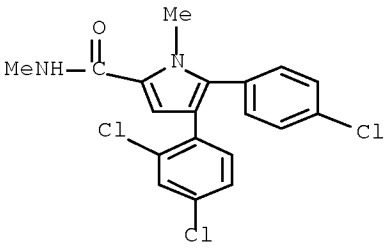


L3 ANSWER 4 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:902048 CAPLUS Full-text
DOCUMENT NUMBER: 147:427173
TITLE: Regioselective Synthesis of Highly Aryl-Substituted Pyrrole Carboxylates as Useful Medicinal Chemistry Leads
AUTHOR(S): Bhatt, Ulhas; Duffy, Bryan C.; Guzzo, Peter R.; Cheng, Leifeng; Elebring, Thomas
CORPORATE SOURCE: Albany Molecular Research, Inc., Albany, NY, USA
SOURCE: Synthetic Communications (2007), 37(16), 2793-2806
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:427173

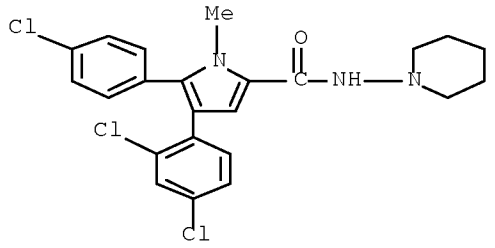
AB The regioselective syntheses of two pharmaceutically relevant pyrrole scaffolds are described. A synthetic route for the preparation of differentially substituted pyrrole-3,4-dicarboxylates is presented and exemplified. This route circumvents some of the problems and limitations associated with previous butynedioic diester condensations and 1,3-dipolar cycloaddn. reactions. A route to the related 4,5-diarylpyrrole-2-carboxylic acid scaffold is also presented. Both routes allow for the regiocontrolled preparation of highly substituted pyrrole pharmacophore cores.

IT 952019-94-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective preparation of aryl-substituted pyrrole-3,4-dicarboxylates and 2-pyrrolecarboxylates)

RN 952019-94-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-N,1-dimethyl- (CA INDEX NAME)



IT 875667-50-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of aryl-substituted pyrrole-3,4-dicarboxylates and 2-pyrrolecarboxylates)
RN 875667-50-8 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-N-1-piperidinyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:874967 CAPLUS Full-text
DOCUMENT NUMBER: 147:257800
TITLE: 3,4-Dihydropyrrolo[1,2-a]pyrazin-1(2H)-ones as melanin concentrating hormone receptor-1 antagonists and their preparation, pharmaceutical compositions and use in the treatment of disease
INVENTOR(S): Zhao, Guohua
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S. Pat. Appl. Publ., 34pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

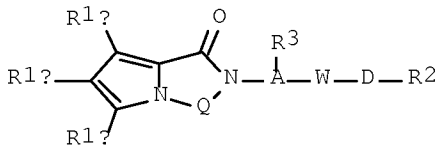
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185097	A1	20070809	US 2007-671150	20070205
WO 2007092416	A2	20070816	WO 2007-US3099	20070206
WO 2007092416	A3	20071101		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1987039	A2	20081105	EP 2007-763593	20070206

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.: US 2006-765530P P 20060206
WO 2007-US3099 W 20070206

OTHER SOURCE(S): MARPAT 147:257800

GI



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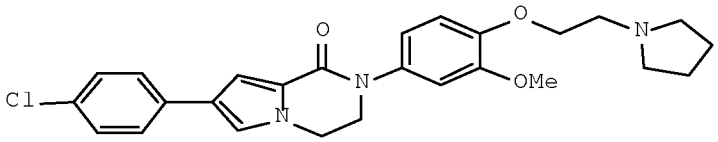


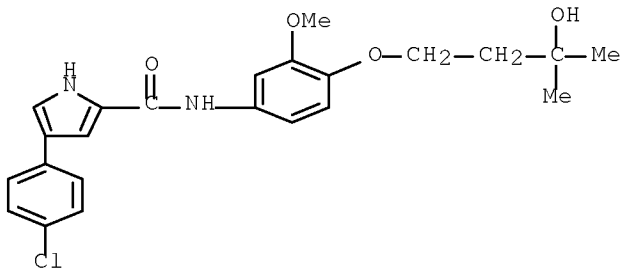
II

AB The application provides compds. of formula I, including all stereoisomers, solvates, prodrugs and pharmaceutically acceptable forms thereof. Addnl., the application provides pharmaceutical compns. containing at least one compound according to formula I and optionally at least one addnl. therapeutic agent. Finally, the application provides methods for treating a patient suffering from an MCHR-1 modulated disease or disorder such as, for example, obesity, diabetes, depression or anxiety by administration of a therapeutically ED of a compound according to formula I. Compds. of formula I wherein A is monocyclic (hetero)aryl and bicyclic heteroaryl; D is a bond, alkyl, cycloalkyl and heterocyclyl; Q is (un)substituted C1-4 alkyl, (un)substituted acetyl, (un)substituted carbonyl-alkyl, CO, COCO, etc.; W is a bond, CO, O, NH and derivs., SO, SO2, SO2NH and derivs., and (un)substituted methylene; R1a, R1b, and R1c are independently H, halo, (un)substituted (hetero)aryl, (un)substituted aryloxy, (un)substituted arylthio, and (un)substituted arylalkylthio; R2 is H, OH, lower alkoxy, hydroxyalkyl, lower cycloalkoxy, OCONH2 and derivs., CN, CONH2 and derivs., etc.; R3 is H, OH, halo, alkoxy, CN, alkyl, perfluoroalkyl, cycloalkyl, etc.; and their pharmaceutically acceptable salts, stereoisomers, solvates, and prodrug esters thereof, are claimed. Example compound II•TFA was prepared by cross-coupling of Me 4-bromo-1H-pyrrole-2-carboxylate with 4-chlorophenylboronic acid; the resulting Me 4-(4-chlorophenyl)-1H-pyrrole-2-carboxylate underwent hydrolysis to give 4-(4-chlorophenyl)-1H-pyrrole-2-carboxylic acid which underwent amidation with 3-methoxy-4-(2-(pyrrolidin-1- yl)ethoxy)benzenamine to give 4-(4-chlorophenyl)-N-(3-methoxy-4-(2- (pyrrolidin-1-yl)ethoxy)phenyl)-1H-pyrrole-2-carboxamide, which underwent cyclization with 1,2-dibromoethane to give compound II•TFA. All the invention compds. were evaluated for their melanin concentrating hormone receptor-1 antagonistic activity.

IT 1057107-73-9
RL: PRPH (Prophetic)
(3,4-Dihydropyrrolo[1,2-a]pyrazin-1(2H)-ones as melanin concentrating hormone receptor-1 antagonists and their preparation, pharmaceutical compositions and use in the treatment of disease)

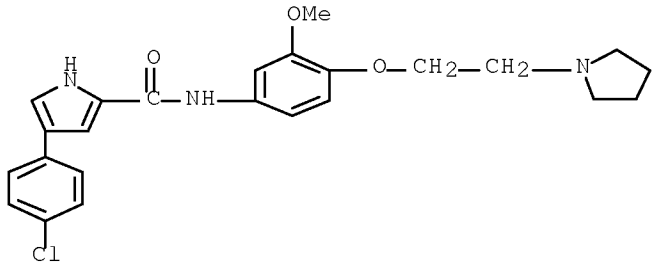
RN 1057107-73-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(3-hydroxy-3-methylbutoxy)-3-methoxyphenyl]- (CA INDEX NAME)

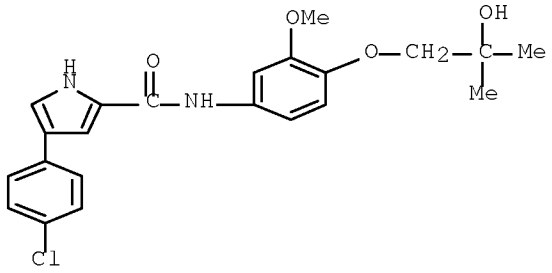


IT 945720-32-1P 945720-37-6P 945720-40-1P
945720-43-4P 945720-44-5P 945720-45-6P
945720-46-7P 945720-47-8P 945720-48-9P
945720-49-0P 945720-50-3P 945720-51-4P
945720-52-5P 945720-55-8P 945720-58-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of dihydropyrrolopyrazinones as melanin concentrating
hormone receptor 1 antagonists useful alone or in combination therapy of MCHR-1 - mediated diseases)

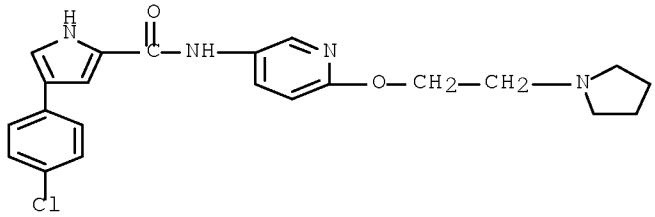
RN 945720-32-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



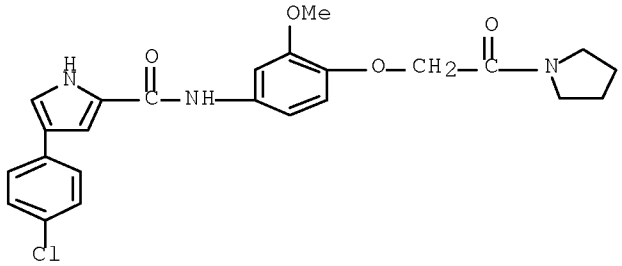
RN 945720-37-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(2-hydroxy-2-methylpropoxy)-3-methoxyphenyl]- (CA INDEX NAME)



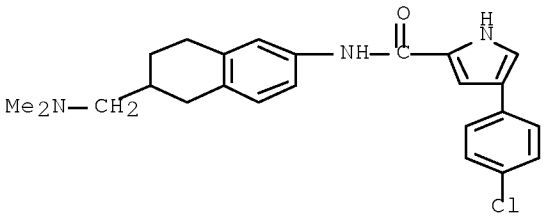
RN 945720-40-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[6-[2-(1-pyrrolidinyl)ethoxy]-3-pyridinyl]- (CA INDEX NAME)



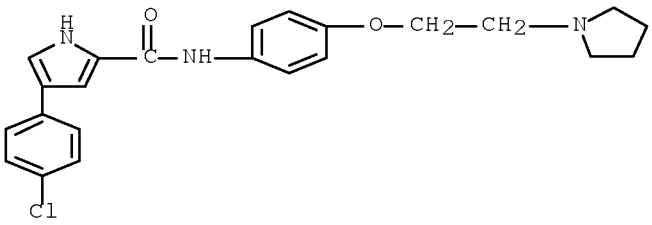
RN 945720-43-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-oxo-2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



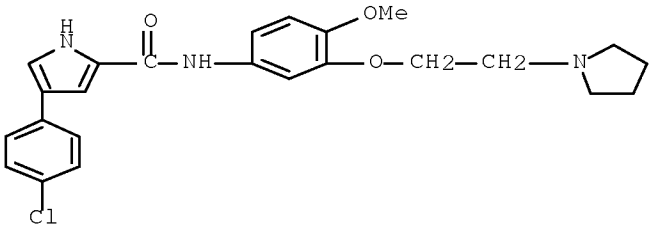
RN 945720-44-5 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[6-[(dimethylamino)methyl]-5,6,7,8-tetrahydro-2-naphthalenyl]- (CA INDEX NAME)



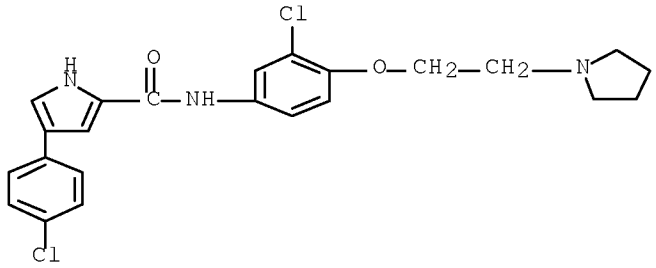
RN 945720-45-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



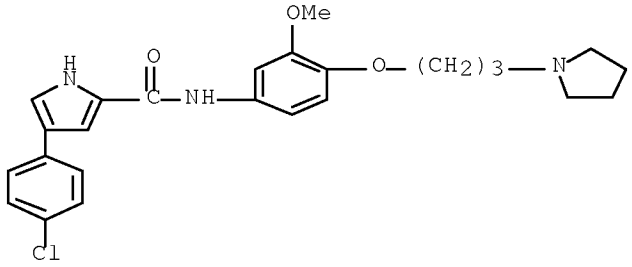
RN 945720-46-7 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-methoxy-3-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



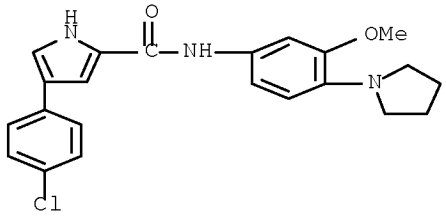
RN 945720-47-8 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-chloro-4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



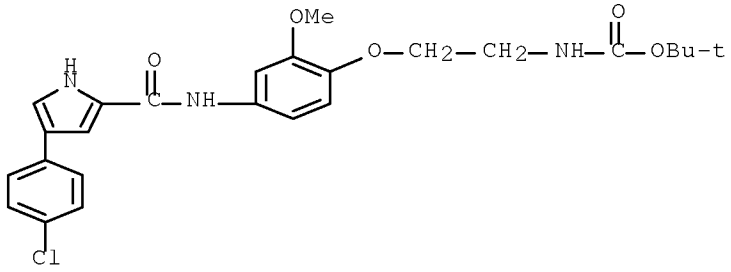
RN 945720-48-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[3-(1-pyrrolidinyl)propoxy]phenyl]- (CA INDEX NAME)



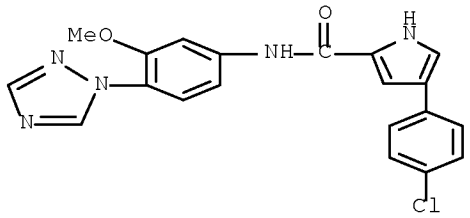
RN 945720-49-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-(1-pyrrolidinyl)phenyl]- (CA INDEX NAME)



RN 945720-50-3 CAPLUS
CN Carbamic acid, N-[2-[4-[[[4-(4-chlorophenyl)-1H-pyrrol-2-yl]carbonyl]amino]-2-methoxyphenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

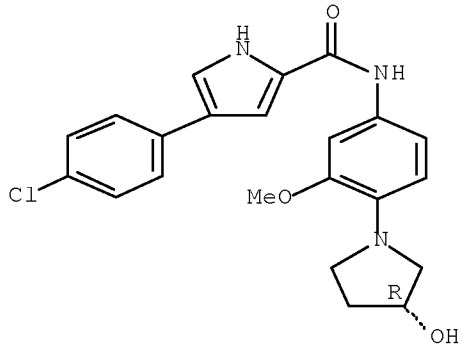


RN 945720-51-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-(1H-1,2,4-triazol-1-yl)phenyl]- (CA INDEX NAME)

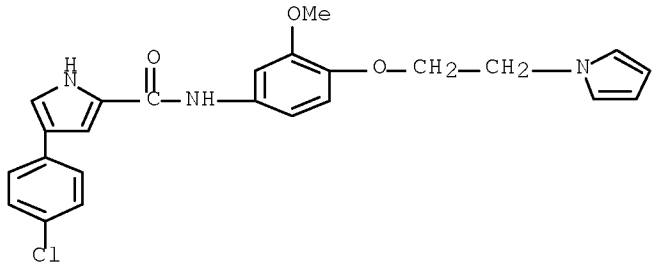


RN 945720-52-5 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-[(3R)-3-hydroxy-1-pyrrolidinyl]-3-methoxyphenyl]- (CA INDEX NAME)

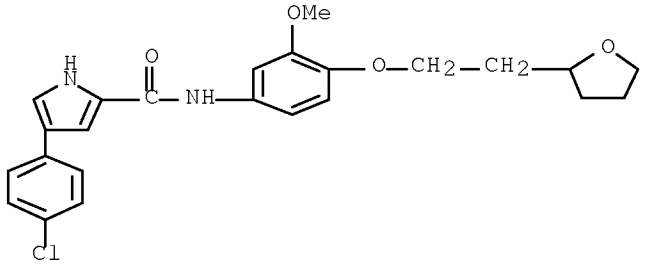
Absolute stereochemistry.



RN 945720-55-8 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(1H-pyrrol-1-yl)ethoxy]phenyl]- (CA INDEX NAME)

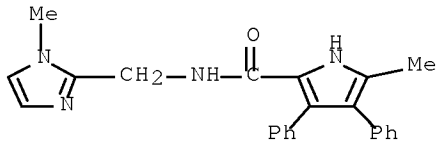


RN 945720-58-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(tetrahydro-2-furanyl)ethoxy]phenyl]- (CA INDEX NAME)



L3 ANSWER 6 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:450172 CAPLUS Full-text
DOCUMENT NUMBER: 147:72319
TITLE: Conformational control of HCl co-transporter: imidazole functionalized isophthalamide vs. 2,6-dicarboxamidopyridine
AUTHOR(S): Gale, Philip A.; Garric, Joachim; Light, Mark E.; McNally, Beth A.; Smith, Bradley D.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2007), (17), 1736-1738
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:72319
AB Replacement of the central isophthalamide core in a synthetic HCl receptor, with a 2,6-dicarboxamidopyridine, leads to a more preorganized mol. structure that exhibits higher chloride affinity and membrane transport flux.
IT 864943-19-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(inclusion reaction; conformational control of HCl co-transporter by imidazole functionalized isophthalamide vs. 2,6-dicarboxamidopyridine)
RN 864943-19-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-

3,4-diphenyl- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1356739 CAPLUS Full-text
DOCUMENT NUMBER: 146:121812
TITLE: 4,5-Diarylpyrrole derivatives, their preparation, and their therapeutic application as cannabinoid CB1 receptor antagonists
INVENTOR(S): Barth, Francis; Congy, Christian; Hortala, Laurent; Rinaldi-Carmona, Murielle
PATENT ASSIGNEE(S): Sanofi Aventis, Fr.
SOURCE: Fr. Demande, 28pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2887548	A1	20061229	FR 2005-6609	20050627
FR 2887548	B1	20070921		
AU 2006263781	A1	20070104	AU 2006-263781	20060622
CA 2610805	A1	20070104	CA 2006-2610805	20060622
WO 2007000505	A2	20070104	WO 2006-FR1416	20060622
WO 2007000505	A3	20071115		
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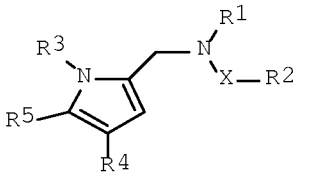
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1899298	A2	20080319	EP 2006-764809	20060622
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
US 20080176924	A1	20080724	US 2007-952224	20071207
IN 2007KN04798	A	20080215	IN 2007-KN4798	20071210
MX 200716383	A	20080307	MX 2007-16383	20071218
KR 2008019641	A	20080304	KR 2007-730262	20071226
CN 101208300	A	20080625	CN 2006-80023067	20071226

NO 2008000458 A 20080124 NO 2008-458 20080124
PRIORITY APPLN. INFO.: FR 2005-6609 A 20050627
WO 2006-FR1416 W 20060622
OTHER SOURCE(S): MARPAT 146:121812
GI



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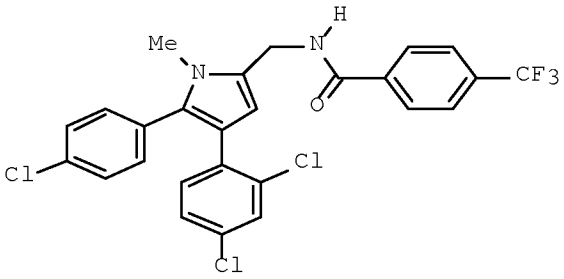
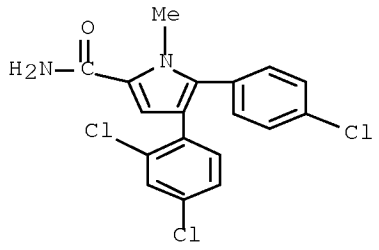


II

AB The invention provides compds. I [X = CO, SO2, or CON(R6); R1 = H or C1-4 alkyl; R2 = C1-7 alkyl, nonarom. C3-12 carbocyclyl optionally substituted by C1-4 alkyl and optionally attached via CH2, (un)substituted Ph, (un)substituted benzyl, benzhydryl, benzhydrylmethyl, 1,2,3,4-tetrahydronaphthalen-2-yl optionally substituted by C1-4 alkyl, heterocycles (pyrrolyl, imidazolyl, pyridyl, pyrazolyl, furyl, or thienyl) optionally substituted by alkyl and/or halo, indol-2-yl, N-methylindol-2-yl; R3 = C1-5 alkyl or C3-7 cycloalkyl; R4, R5 = (un)substituted Ph; R6 = H or C1-4 alkyl; including bases, acid addition salts, hydrates, and/or solvates]. Also provided are a process for preparing I, and therapeutic applications of I. Claimed uses include the treatment or prevention of appetite disorders, metabolic disorders, gastrointestinal diseases, inflammatory phenomena, immune system disorders, psychotic disorders, alc. dependence, and nicotine dependence. Eighteen compds. I are described in detail, 13 of which were prepared by combinatorial methods. For instance, the ester Me 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1H- pyrrole-2-carboxylate (prepared in 5 steps) underwent a sequence of 4 steps (hydrolysis, amidation, reduction of the carboxamide to a methylamine, and amidation of the amine with the corresponding acid chloride) to give invention compound II. Compds. I have very good in vitro affinity for cannabinoid CB1 receptors, with IC50 ≤ 5+10-7M. The antagonist nature of compds. I was demonstrated by adenylate-cyclase inhibition models, and toxicity was compatible with therapeutic use (no data).

IT 918294-12-9P, 5-(4-Chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-1H-pyrrole-2-carboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of diarylpyrrole derivs. as cannabinoid CB1 receptor antagonists)

RN 918294-12-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:699903 CAPLUS Full-text
DOCUMENT NUMBER: 145:145709
TITLE: Preparation of heterocyclic carboxamide compounds as steroid nuclear receptors ligands
INVENTOR(S): Flatt, Brenton; Gu, Xiao-Hui; Martin, Richard; Mohan, Raju; Murphy, Brett; Nyman, Michael C.; Stevens, William C., Jr.; Wang, Tie-Lin
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 196 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

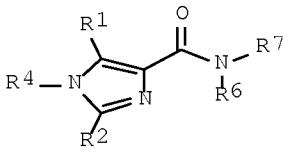
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006076202	A1	20060720	WO 2006-US319	20060106
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006205220	A1	20060720	AU 2006-205220	20060106
CA 2593156	A1	20060720	CA 2006-2593156	20060106
EP 1844020	A1	20071017	EP 2006-717506	20060106
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
JP 2008526869	T	20080724	JP 2007-550462	20060106

PRIORITY APPLN. INFO.: US 2005-642839P P 20050110

WO 2006-US319 W 20060106

OTHER SOURCE(S): MARPAT 145:145709

GI



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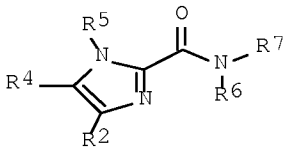


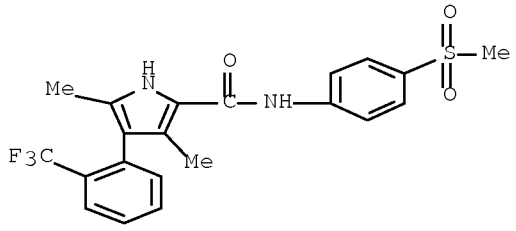
II

AB Imidazole-4-carboxamides (I) and imidazole-2-carboxamide (II) [R1, R2 = H, cyano, halo, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R5 = H, each alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R4 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R6 = H; R7 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl] as single isomers, mixture of isomers, or as racemic mixts. of isomers or as solvates or polymorphs or as prodrugs or metabolites or as pharmaceutically acceptable salts thereof are prepared These compds. are useful in modulating the activity of steroid nuclear receptors and thereby for the treatment of a disease, or disorder mediated by, or otherwise affected by one or more steroid nuclear receptors (in particular mineralocorticoid receptor), or in which steroid nuclear receptor activity is implicated. The above disease or disorder is related to cancer, infertility, one or more metabolic syndromes, bone or cartilage dysfunction, immune dysfunction, cognitive dysfunction, high blood pressure, heart disease, renal disease, fibrosis, epidermal dysfunction, or muscle wasting. Thus, to a stirred mixture of 1,4-dimethyl-5-(2-phenoxyphenyl)-1H-imidazole-2-carboxylic acid Et ester (202 mg, 0.60 mmol) and 4-methanesulfonylaniline (136 mg, 0.80 mmol) in toluene (5 mL, anhydrous) was added dropwise Me3Al (2.0 M in toluene, 0.4 mL, 0.8 mmol) under N at ambient temperature and the resulting mixture was stirred at 100° in a sealed vial for 10 h to give, after silica gel chromatog., 1,4-dimethyl-5-(2-phenoxyphenyl)-1H-imidazole-2-carboxylic acid (4-methanesulfonylphenyl)amide (III). III showed antagonist activity against mineralocorticoid receptor with IC50 of <0.5 μM which was ten-fold greater than the antagonist activity against androgen receptor (AR), estrogen receptor α (ERα), glucocorticoid receptor (GR), and progesterone receptor (PR).

IT 880779-28-2P, 3,5-Dimethyl-4-(2-trifluoromethylphenyl)-1H-pyrrole-2-carboxylic acid N-(4-methylsulfonylphenyl)amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolecarboxamides as modulators of steroid nuclear receptors)

RN 880779-28-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3,5-dimethyl-N-[4-(methylsulfonyl)phenyl]-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



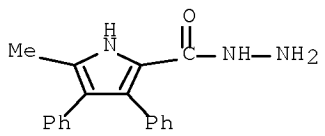
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:640343 CAPLUS Full-text
DOCUMENT NUMBER: 145:188387
TITLE: Pyrrolylamidourea based anion receptors
AUTHOR(S): Evans, Louise S.; Gale, Philip A.; Light, Mark E.; Quesada, Roberto
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: New Journal of Chemistry (2006), 30(7), 1019-1025
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:188387

AB The anion binding behavior of a number of pyrrolylamidourea and thiourea compds. have been studied in DMSO solution Mono-amidothioureapyrrole compds. were found to be deprotonated by basic anions such as fluoride, acetate, benzoate or dihydrogenphosphate with the structure of the deprotonated species elucidated by X-ray crystallog. 2,5-Bis(amidourea)pyrroles were synthesized and found to be effective anion receptors for a range of putative anionic guests.

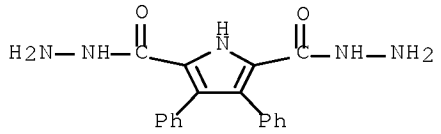
IT 884529-86-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystallog.; addition to aryl isocyanate; pyrrolylamidourea based anion receptors)

RN 884529-86-6 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, hydrazide (CA INDEX NAME)



IT 902141-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystallog.; addition to aryl isocyanate; pyrrolylamidourea based anion

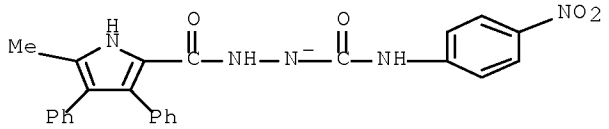
receptors)
RN 902141-41-7 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-, 2,5-dihydrazide (CA INDEX NAME)



IT 902141-43-9
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(crystallog.; pyrrolylamidourea based anion receptors)
RN 902141-43-9 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, 5-methyl-3,4-diphenyl-1H-pyrrole-2-carboxylic acid hydrazide (1:1) (CA INDEX NAME)

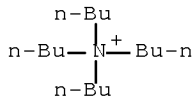
CM 1

CRN 902141-42-8
CMF C25 H20 N5 O4



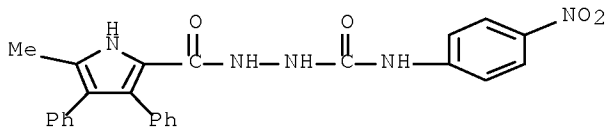
CM 2

CRN 10549-76-5
CMF C16 H36 N

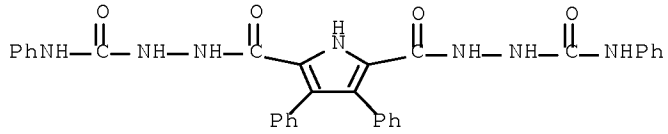


IT 884529-83-3P 902141-33-7P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystallog.; pyrrolylamidourea based anion receptors)
RN 884529-83-3 CAPLUS

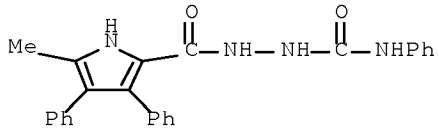
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[[(4-nitrophenyl)amino]carbonyl]hydrazide (CA INDEX NAME)



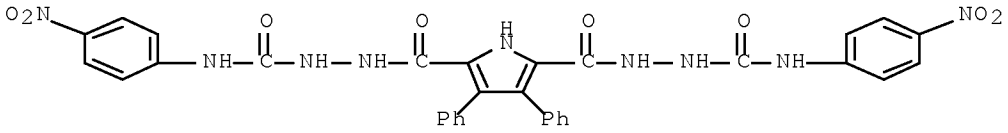
RN 902141-33-7 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-,
2,5-bis[2-[(phenylamino)carbonyl]hydrazide] (CA INDEX NAME)



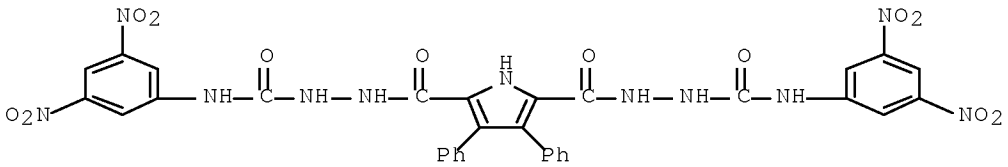
IT 884529-82-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(no association with anions; pyrrolylamidourea based anion receptors)
RN 884529-82-2 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[(phenylamino)carbonyl]hydrazide (CA INDEX NAME)



IT 902141-35-9P 902141-37-1P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(pyrrolylamidourea based anion receptors)
RN 902141-35-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-,
2,5-bis[2-[[(4-nitrophenyl)amino]carbonyl]hydrazide] (CA INDEX NAME)

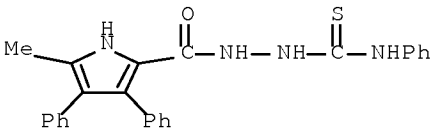


RN 902141-37-1 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-, 2,5-bis[2-[[(3,5-dinitrophenyl)amino]carbonyl]hydrazide] (CA INDEX NAME)

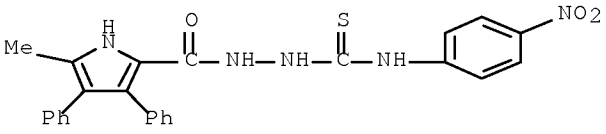


IT 884529-84-4P 884529-85-5P
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(pyrrolylamidourea based anion receptors)

RN 884529-84-4 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[(phenylamino)thioxomethyl]hydrazide (CA INDEX NAME)



RN 884529-85-5 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[[(4-nitrophenyl)amino]thioxomethyl]hydrazide (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:332235 CAPLUS Full-text
DOCUMENT NUMBER: 144:350539
TITLE: Preparation of pyrrolecarboxamide derivatives as mineralocorticoid receptor antagonists for use against cancer and other disorders
INVENTOR(S): Canne Bannen, Lynne; Chen, Jeff; Dalrymple, Lisa Esther; Flatt, Brenton T.; Forsyth, Timothy Patrick; Gu, Xiao-Hu; Mac, Morrison B.; Mann, Larry W.; Mann, Grace; Martin, Richard; Mohan, Raju; Murphy, Brett; Nyman, Michael Charles; Stevens, William C., Jr.; Wang, Tie-Lin; Wong, Yong; Wu, Jason H.
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 477 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2006012642	A2	20060202	WO 2005-US26916		20050730
WO 2006012642	A3	20060727			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
AU 2005266890	A1	20060202	AU 2005-266890		20050730
CA 2573426	A1	20060202	CA 2005-2573426		20050730
EP 1773768	A2	20070418	EP 2005-803281		20050730
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CN 101006052	A	20070725	CN 2005-80026842		20050730
BR 2005013677	A	20071127	BR 2005-13677		20050730
JP 2008508308	T	20080321	JP 2007-523832		20050730
IN 2007DN00605	A	20070817	IN 2007-DN605		20070123
NO 2007000910	A	20070426	NO 2007-910		20070216
KR 2007045283	A	20070502	KR 2007-704302		20070223
US 20080234270	A1	20080925	US 2007-572962		20071203
PRIORITY APPLN. INFO.:			US 2004-592439P	P	20040730
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			WO 2005-US26916	W	20050730

OTHER SOURCE(S): MARPAT 144:350539
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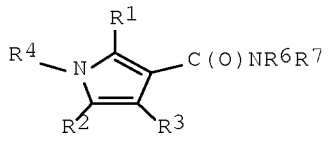


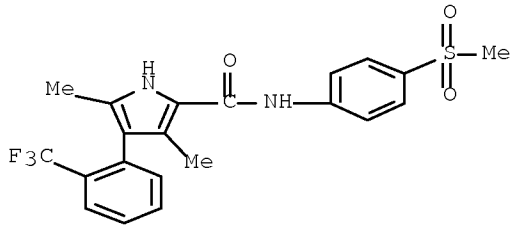
I

AB Pyrrolecarboxamide derivs. (shown as I; other Markush structures for pyrrolecarboxamides are defined in the claims; variables defined below; e.g. 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole-3- carboxylic acid N-[4-(sulfamoyl)phenyl]amide (II)), compns. and methods for modulating the activity of receptors are provided. In particular compds. and compns. are provided for modulating the activity of receptors and for the treatment, prevention, or amelioration of ≥1 symptoms of disease or disorder directly or indirectly related to the activity of the receptors. Semiquant. IC50 values for antagonist activity of 23 examples of I are tabulated and compared to the activity of the Spironolactone control. For I: R1 and R2 = H, halo, cyano, or (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocyclylalkyl, or -OR9, -SR9, -N(R9)2, -C(O)OR9 or -C(O)N(R9)2; R3 = H, halo, cyano, (un)substituted alkyl, (un)substituted alkenyl or (un)substituted alkynyl; R4 is H, -C(O)R9, -S(O)2R9, or (un)substituted alkyl, alkenyl or alkynyl, or R4 is (un)substituted cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; R6 is H or (un)substituted alkyl; R7 is (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; addnl. details are given in the claims. Although the methods of preparation are not claimed, prepns. and/or characterization data for many examples of I are included. For example, II was prepared in 5 steps (50, 37, 62, 64, and 66 % yields, resp.) starting with preparation of 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole from 4-fluoro-2-(trifluoromethyl)aniline and 2,5-hexanedione, followed by preparation of the following intermediates: 1-(4-fluoro-2-trifluoromethylphenyl)-2,5-dimethyl-1H-pyrrole-3- carboxaldehyde, 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H- pyrrole-3-carboxylic acid, and 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5- dimethyl-1H-pyrrole-3-carbonyl chloride and finally amide formation with sulfanilamide.

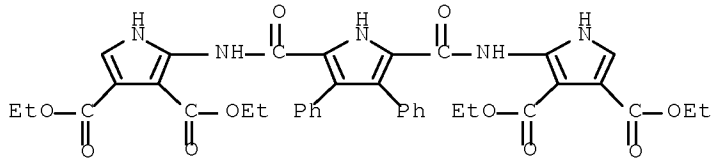
IT 880779-28-2P, 3,5-Dimethyl-4-(2-trifluoromethylphenyl)-1H-pyrrole-2-carboxylic acid N-(4-methylsulfonylphenyl)amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrrolecarboxamide derivs. as mineralocorticoid receptor antagonists for use against cancer and other disorders)

RN 880779-28-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3,5-dimethyl-N-[4-(methylsulfonyl)phenyl]-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L3 ANSWER 11 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:239131 CAPLUS Full-text
DOCUMENT NUMBER: 144:467975
TITLE: Synthesis and Anion Binding Properties of N,N'-Bispyrrol-2-yl-2,5-diamidopyrrole
AUTHOR(S): Sessler, Jonathan L.; Pantos, G. Dan; Gale, Philip A.; Light, Mark E.
CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-0165, USA
SOURCE: Organic Letters (2006), 8(8), 1593-1596
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:467975
AB A bispyrrol-2-yl-2,5-diamidopyrrole has been synthesized and shown to have a significantly higher affinity for oxo-anions than previous generation 2,5-diamidopyrroles.
IT 886589-23-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anion binding of a 3,4-diphenyl-2,5-bis(2-pyrrolylcarbamoyl)pyrrole)
RN 886589-23-7 CAPLUS
CN 1H-Pyrrole-3,4-dicarboxylic acid, 2,2'-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis-, tetraethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:160694 CAPLUS Full-text
DOCUMENT NUMBER: 144:424677
TITLE: Anion binding vs. deprotonation in colorimetric

pyrrolylamidothiourea based anion sensors

AUTHOR(S): Evans, Louise S.; Gale, Philip A.; Light, Mark E.; Quesada, Roberto

CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (9), 965-967
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

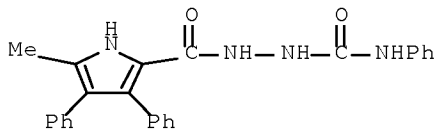
OTHER SOURCE(S): CASREACT 144:424677

AB A pyrrolylamidothiourea deprotonates in the presence of one equivalent of not only fluoride, but also acetate, benzoate or dihydrogen phosphate in DMSO solution with structural studies using synchrotron radiation confirming thiourea deprotonation in the solid state.

IT 884529-82-2P 884529-83-3P 884529-84-4P
884529-85-5P
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(anion binding vs. deprotonation in colorimetric pyrrolylamidothiourea based anion sensors)

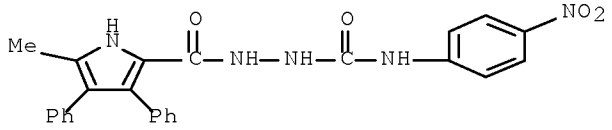
RN 884529-82-2 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[(phenylamino)carbonyl]hydrazide (CA INDEX NAME)



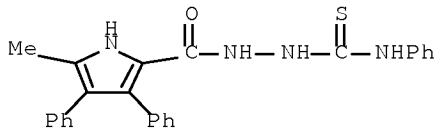
RN 884529-83-3 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[[(4-nitrophenyl)amino]carbonyl]hydrazide (CA INDEX NAME)

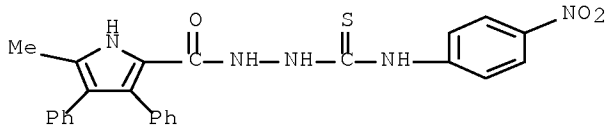


RN 884529-84-4 CAPLUS

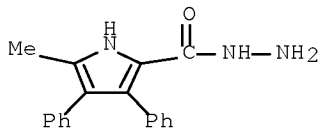
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[(phenylamino)thioxomethyl]hydrazide (CA INDEX NAME)



RN 884529-85-5 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, 2-[[(4-nitrophenyl)amino]thioxomethyl]hydrazide (CA INDEX NAME)



IT 884529-86-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use in preparation of pyrrolylamidothiourea)
RN 884529-86-6 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, hydrazide (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:128973 CAPLUS Full-text
DOCUMENT NUMBER: 144:440844
TITLE: Anion binding properties of diamide derivatives of pyrrole-2, 5-diacetic acid in different solvents
AUTHOR(S): Li, Rong-qing; Gao, Zhi-hong
CORPORATE SOURCE: Department of Chemistry, Jiangsu Province Key Laboratory for Chemistry of Low-Dimensional Materials, Huaiyin Teachers College, Huaian, 223300, Peop. Rep. China
SOURCE: Henan Shifan Daxue Xuebao, Ziran Kexueban (2005), 33(4), 80-82, 125
CODEN: HESKER; ISSN: 1000-2367
PUBLISHER: Henan Shifan Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal

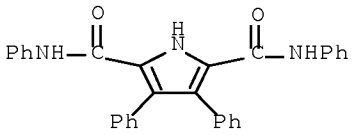
LANGUAGE: Chinese

AB The anion binding properties of diamide derivs. of pyrrole-2,5-diacetic acid in different solvents were investigated, using 1H NMR titration techniques. These derivs. are shown to be effective receptors for oxo-anions in acetonitrile-d3 solution, with comparable binding affinities to those found for simple pyrrole-2,5-dicarboxamides, despite possessing a more flexible hydrogen bonding array. However, they display reduced affinities for all the anions studied in a more competitive solvent, DMSO-d6, as compared to the association consts. measured in acetonitrile-d3.

IT 365214-50-2
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(anion binding properties of diamide derivs. of pyrrole-2, 5-diacetic acid in different solvents studied by using 1H NMR titration techniques)

RN 365214-50-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



L3 ANSWER 14 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:126304 CAPLUS Full-text

DOCUMENT NUMBER: 144:212649

TITLE: Preparation of 4,5-diphenylpyrrole-2-carboxamide derivatives as antagonists of CB1 cannabinoid receptors and their therapeutic application

INVENTOR(S): Barth, Francis; Congy, Christian; Hortala, Laurent; Rinaldi Carmona, Murielle

PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.

SOURCE: Fr. Demande, 26 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2874012	A1	20060210	FR 2004-8773	20040809
FR 2874012	B1	20080822		
AU 2005279086	A1	20060309	AU 2005-279086	20050802
CA 2576717	A1	20060309	CA 2005-2576717	20050802
WO 2006024777	A1	20060309	WO 2005-FR2015	20050802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 1781636	A1	20070509	EP 2005-796087		20050802
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU					
CN 101014588	A	20070808	CN 2005-80030251		20050802
JP 2008509202	T	20080327	JP 2007-525320		20050802
BR 2005014235	A	20080603	BR 2005-14235		20050802
US 20070149596	A1	20070628	US 2007-625616		20070122
US 7381727	B2	20080603			
IN 2007KN00337	A	20070706	IN 2007-KN337		20070131
MX 200701383	A	20070419	MX 2007-1383		20070202
NO 2007001209	A	20070305	NO 2007-1209		20070305
KR 2007054649	A	20070529	KR 2007-705467		20070308
US 20080194581	A1	20080814	US 2008-102412		20080414
PRIORITY APPLN. INFO.:			FR 2004-8773	A	20040809
			WO 2005-FR2015	W	20050802
			US 2007-625616	A1	20070122

OTHER SOURCE(S): MARPAT 144:212649
GI

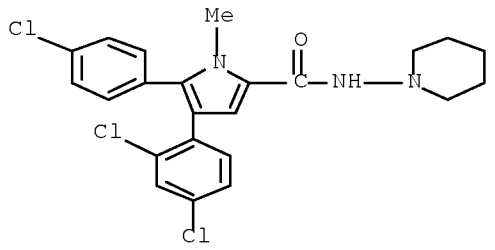
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl; R2 = alkyl, 1,2,3,4-tetrahydronaphthalen-1-yl, 1,2,3,4-tetrahydronaphthalen-2-yl, (un)substituted heterocyclyl, phenylalkylene, etc.; or NR1R2 = (un)substituted piperazin-1-yl, 1,4-diazepan-1-yl, piperidin-1-yl, pyrrolidin-1-yl; R3-R8 = independently H, halo, alkyl, alkoxy, CF3, etc.; R9 = alkyl; and their free bases, and their acid addition salts, hydrates and solvates] were prepared as antagonists of CB1 cannabinoid receptors and for treatment of the diseases it implies. For instance, II (m.p. = 165°) was prepared in 7 steps via cyclization of alkyne III (preparation given) in the presence of I2/K2CO3, Pd-coupling with (2,4-dichlorophenyl)boronic acid, Ts-deprotection, alkylation of the pyrrole IV with MeI in the presence of K2CO3/ester hydrolysis (ester not isolated) and amidation of the acid with N-aminopiperidine. I exhibited an excellent affinity in vitro (IC50 ≤ 5•10-7 M) for the CB1 cannabinoid receptors. Thus, I are useful for treating psychosis, appetite and gastrointestinal disorders, smoking and alc. cessation, etc.

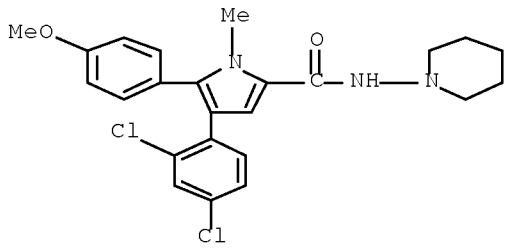
IT 875667-50-8P, 5-(4-Chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-N-(piperidin-1-yl)-1H-pyrrole-2-carboxamide 875667-52-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrrole carboxamide derivs. as antagonists of CB1 cannabinoid receptors)

RN 875667-50-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-N-1-piperidinyl- (CA INDEX NAME)

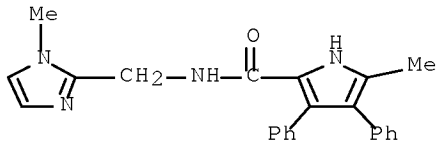


RN 875667-52-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(2,4-dichlorophenyl)-5-(4-methoxyphenyl)-1-methyl-N-1-piperidinyl- (CA INDEX NAME)

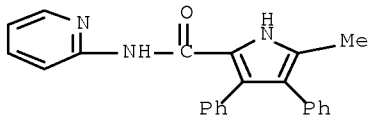


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

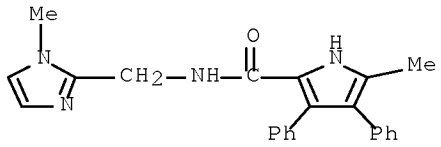
L3 ANSWER 15 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:104702 CAPLUS Full-text
DOCUMENT NUMBER: 144:462886
TITLE: Co-transport of H+/Cl- by a synthetic prodigiosin mimic. [Erratum to document cited in CA143:300973]
AUTHOR(S): Gale, Philip A.; Light, Mark E.; McNally, Beth; Navakhun, Korakot; Sliwinski, Kate E.; Smith, Bradley D.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (2), 226
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structural formula for compound 2 on page 3773 was incorrect. The correct version of compound 2 is given.
IT 864943-19-1P
RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cotransport of H+/Cl- by synthetic prodigiosin mimic (Erratum))
RN 864943-19-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-3,4-diphenyl- (CA INDEX NAME)



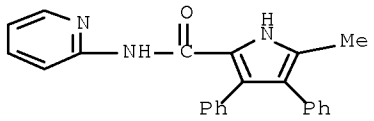
IT 864943-20-4P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cotransport of H+/Cl- by synthetic prodigiosin mimic (Erratum))
RN 864943-20-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-3,4-diphenyl-N-2-pyridinyl- (CA INDEX NAME)



L3 ANSWER 16 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:645311 CAPLUS Full-text
DOCUMENT NUMBER: 143:300973
TITLE: Co-transport of H+/Cl- by a synthetic prodigiosin mimic
AUTHOR(S): Gale, Philip A.; Light, Mark E.; McNally, Beth; Navakhun, Korakot; Sliwinski, Kate E.; Smith, Bradley D.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (30), 3773-3775
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:300973
AB An amidopyrrole with appended imidazole group can bind and co-transport H+/Cl- across vesicle membranes much more effectively than an analog with an appended pyridyl group.
IT 864943-19-1P
RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cotransport of H+/Cl- by synthetic prodigiosin mimic)
RN 864943-19-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-3,4-diphenyl- (CA INDEX NAME)



IT 864943-20-4P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cotransport of H+/Cl- by synthetic prodigiosin mimic)
RN 864943-20-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-3,4-diphenyl-N-2-pyridinyl- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:469894 CAPLUS Full-text
DOCUMENT NUMBER: 143:7592
TITLE: Preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors.
INVENTOR(S): Finsinger, Dirk; Buchstaller, Hans-Peter; Burgdorf, Lars; Wiesner, Matthias; Amendt, Christiane; Grell, Matthias; Sirrenberg, Christian; Zenke, Frank
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 32 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10354060	A1	20050602	DE 2003-10354060	20031119
AU 2004291255	A1	20050602	AU 2004-291255	20041026
CA 2546334	A1	20050602	CA 2004-2546334	20041026
WO 2005049603	A1	20050602	WO 2004-EP12076	20041026

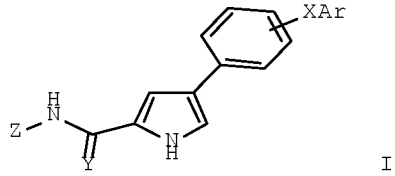
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1685125	A1	20060802	EP 2004-790859		20041026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
CN 1882571	A	20061220	CN 2004-80034345		20041026
BR 2004016690	A	20070130	BR 2004-16690		20041026
JP 2007511553	T	20070510	JP 2006-540216		20041026
IN 2006KN00936	A	20070420	IN 2006-KN936		20060417
MX 2006PA05478	A	20060811	MX 2006-PA5478		20060515
KR 2006118492	A	20061123	KR 2006-709552		20060517
US 20070149594	A1	20070628	US 2006-579825		20060517
PRIORITY APPLN. INFO.:			DE 2003-10354060	A	20031119
			WO 2004-EP12076	W	20041026

OTHER SOURCE(S): MARPAT 143:7592

GI



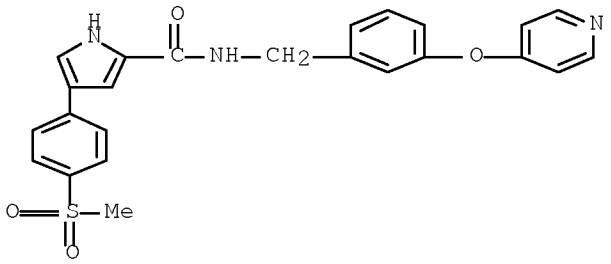
I

AB Title compds. [I; Ar = (substituted) Ph, naphthyl, biphenyl, heterocyclyl; X = O, S, (CH2)n, CO, (CH2)nO, (CH2)nNH, etc.; n = 1-3; Y = O, S, CHNO2, C(CN)2, NR4; R4 = H, cyano, OH, etc.; Z = Ar, ArXAr, CH2Ar, CH2ArXAr; Ar = (substituted) Ph], were prepared as Raf kinase inhibitors (no data). Thus, 4-(PhCH2O)C6H4CH2CO2H, DMF, and POCl3 were heated together at 70° for 4 h followed by cooling and addition of ice water and aqueous NaClO4 to give 98% [2-(4-benzyloxyphenyl)-3-dimethylaminoallylidene]dimethylammonium perchlorate. This was refluxed 24 h with glycine Et ester hydrochloride in EtOH containing 20% NaOEt to give 91% Et 4-(4-benzyloxyphenyl)-1H-pyrrole-2-carboxylate. Hydrogenolysis of the latter in EtOAc over Pd/C gave 91% Et 4-(4-hydroxyphenyl)-1H-pyrrole-2-carboxylate. This was heated with 4-chloropyridine-2-carboxylic acid N-methylamide at 160° for 48 h to give 40% Et 4-[4-(2-methylcarbamoylpyridin-4-yloxy)phenyl]-1H-pyrrole-2- carboxylate. Saponification with 2N NaOH in EtOH at 60° for 16 h followed by acidification with HCl gave 85% free acid, which was stirred 48 h in DMF with 5-amino-2-chlorobenzotrifluoride, N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride, and 1-hydroxybenzotriazole hydrate to give 17% 4-[4-[5-(4-chloro-3-trifluoromethylphenylcarbamoyl)-1H-pyrrol-3- yl]phenoxy]pyridine-2-carboxylic acid N-methylamide.

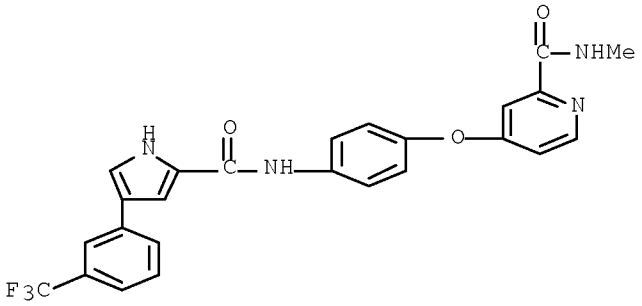
IT 1073641-53-8 1073641-54-9 1073641-55-0
1073641-56-1 1073641-58-3 1073641-59-4
1073641-60-7 1073641-61-8 1073641-62-9
1073641-63-0 1073641-64-1
RL: PRPH (Prophetic)
(Preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors.)

RN 1073641-53-8 CAPLUS

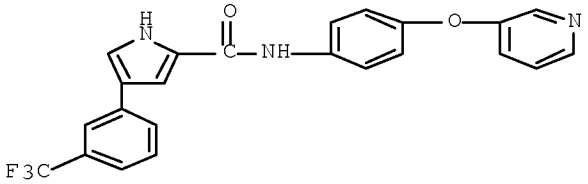
CN 1H-Pyrrole-2-carboxamide, 4-[4-(methylsulfonyl)phenyl]-N-[[3-(4-pyridinyloxy)phenyl]methyl]- (CA INDEX NAME)



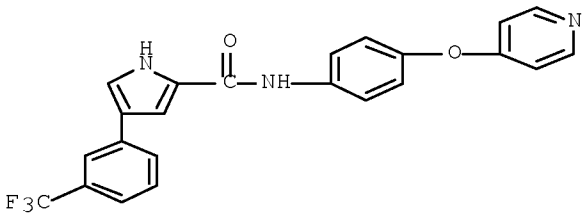
RN 1073641-54-9 CAPLUS
CN 2-Pyridinecarboxamide, N-methyl-4-[4-[[[4-[3-(trifluoromethyl)phenyl]-1H-pyrrol-2-yl]carbonyl]amino]phenoxy]- (CA INDEX NAME)



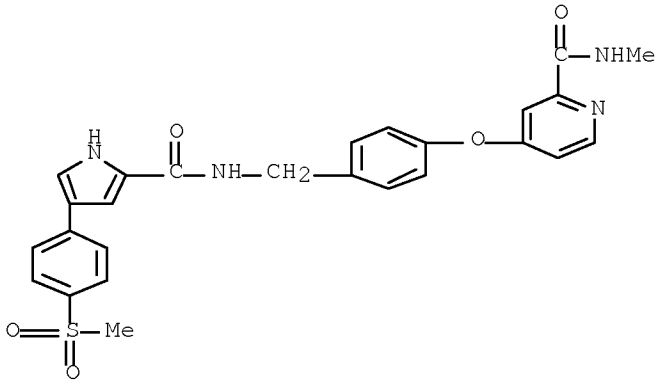
RN 1073641-55-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-[4-(3-pyridinyloxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



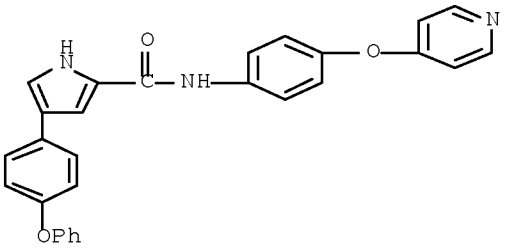
RN 1073641-56-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-[4-(4-pyridinyloxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



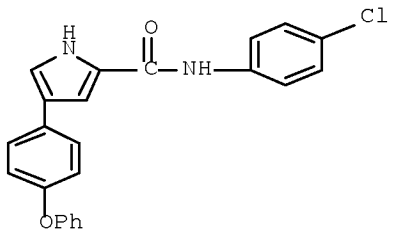
RN 1073641-58-3 CAPLUS
CN 2-Pyridinecarboxamide, N-methyl-4-[4-[[[[4-[4-(methylsulfonyl)phenyl]-1H-pyrrol-2-yl]carbonyl]amino]methyl]phenoxy]- (CA INDEX NAME)



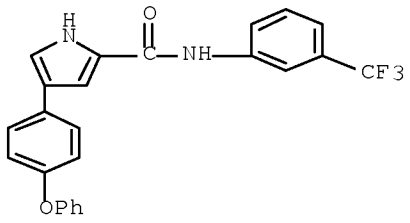
RN 1073641-59-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-phenoxyphenyl)-N-[4-(4-pyridinyloxy)phenyl]- (CA INDEX NAME)



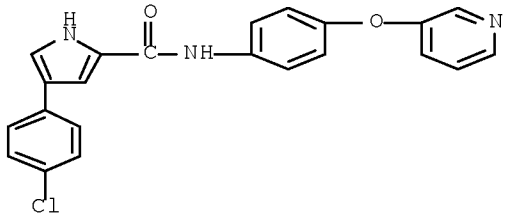
RN 1073641-60-7 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-(4-chlorophenyl)-4-(4-phenoxyphenyl)- (CA INDEX NAME)



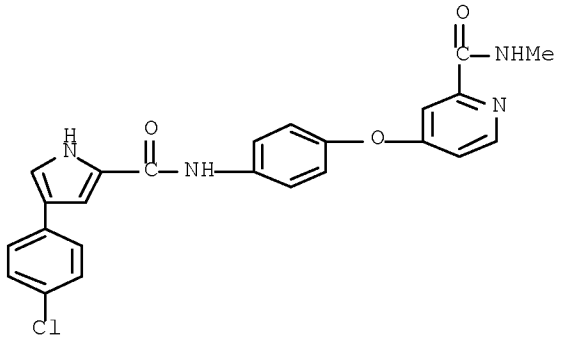
RN 1073641-61-8 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-phenoxyphenyl)-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



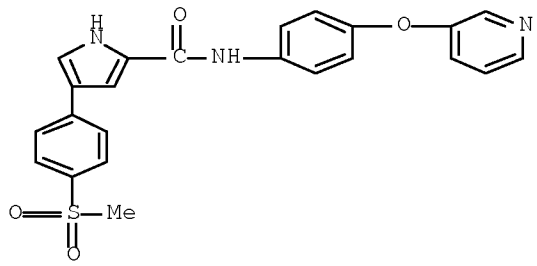
RN 1073641-62-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)



RN 1073641-63-0 CAPLUS
CN 2-Pyridinecarboxamide, 4-[4-[[[4-(4-chlorophenyl)-1H-pyrrol-2-yl]carbonyl]amino]phenoxy]-N-methyl- (CA INDEX NAME)

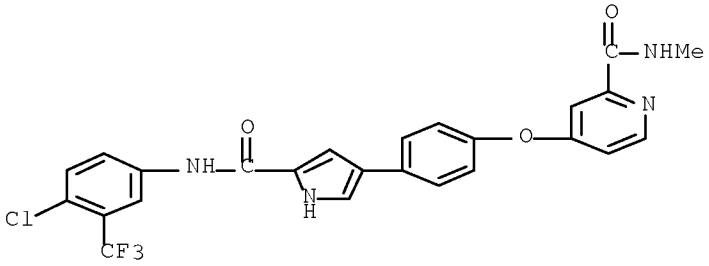


RN 1073641-64-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(methylsulfonyl)phenyl]-N-[4-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)

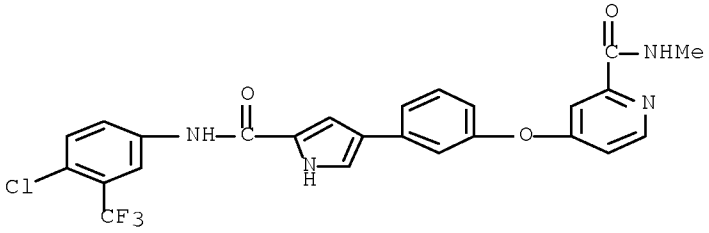


IT 852455-19-7P 852455-20-0P 852455-21-1P
852455-22-2P 852455-23-3P 852455-24-4P
852455-25-5P 852455-26-6P 852455-27-7P
852455-28-8P 852455-29-9P 852455-30-2P
852455-31-3P 852455-32-4P 852455-33-5P
852455-34-6P 852455-35-7P 852455-36-8P
852455-37-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors)

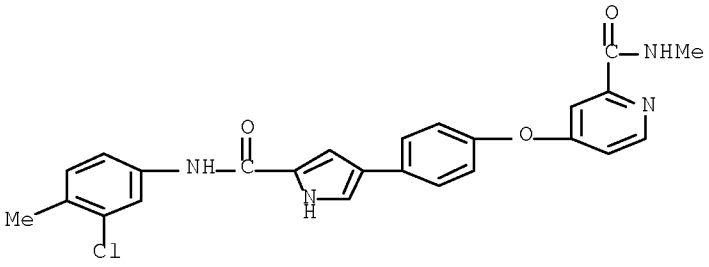
RN 852455-19-7 CAPLUS
CN 2-Pyridinecarboxamide, 4-[4-[5-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



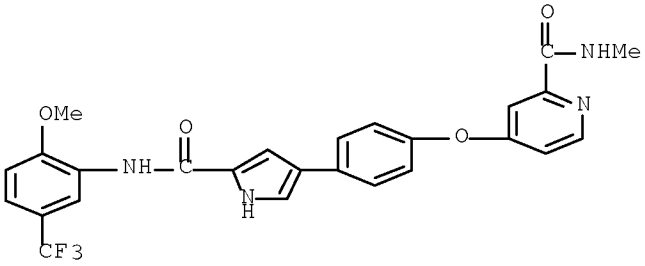
RN 852455-20-0 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



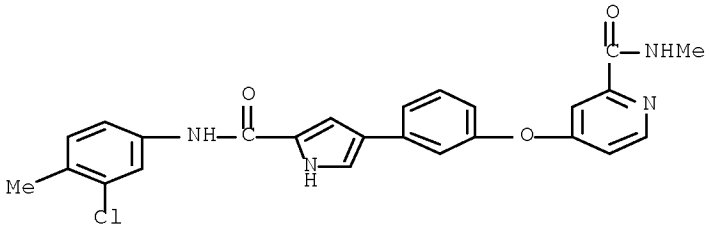
RN 852455-21-1 CAPLUS
CN 2-Pyridinecarboxamide, 4-[4-[5-[[(3-chloro-4-methylphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



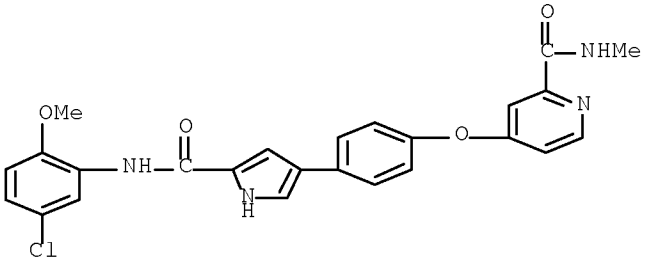
RN 852455-22-2 CAPLUS
CN 2-Pyridinecarboxamide, 4-[4-[5-[[[2-methoxy-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



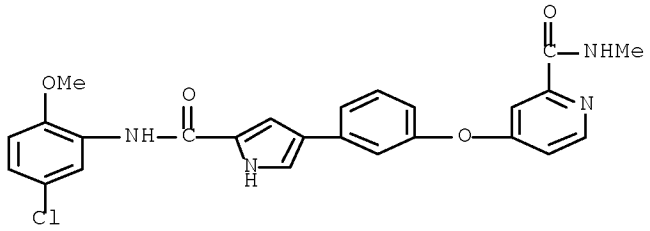
RN 852455-23-3 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[(3-chloro-4-methylphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



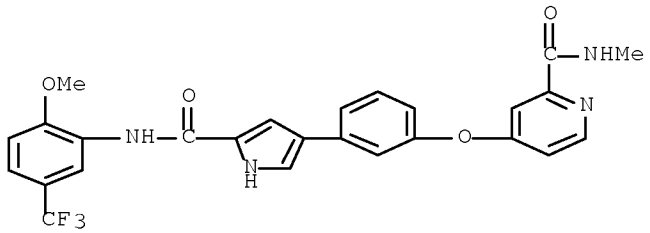
RN 852455-24-4 CAPLUS
CN 2-Pyridinecarboxamide, 4-[4-[5-[[(5-chloro-2-methoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



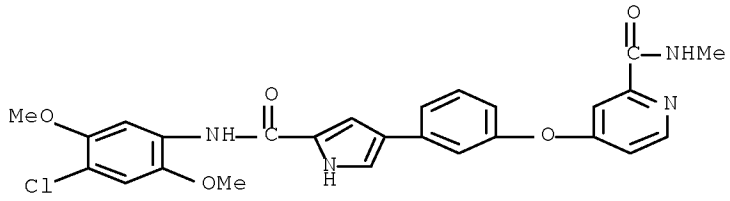
RN 852455-25-5 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[(5-chloro-2-methoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



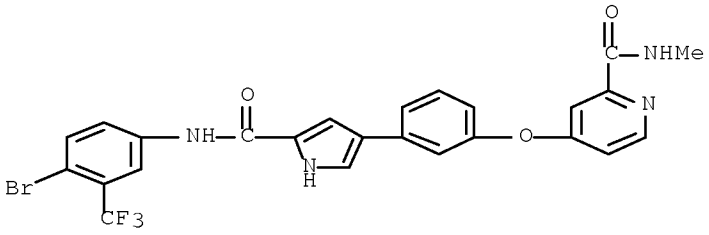
RN 852455-26-6 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-methoxy-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



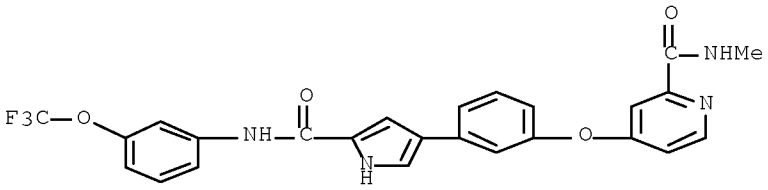
RN 852455-27-7 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[(4-chloro-2,5-dimethoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



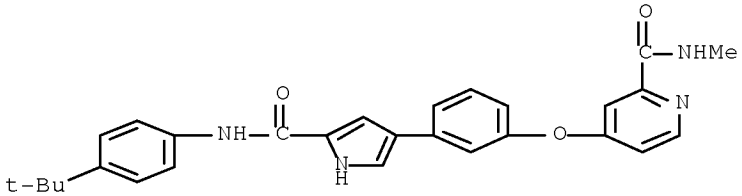
RN 852455-28-8 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



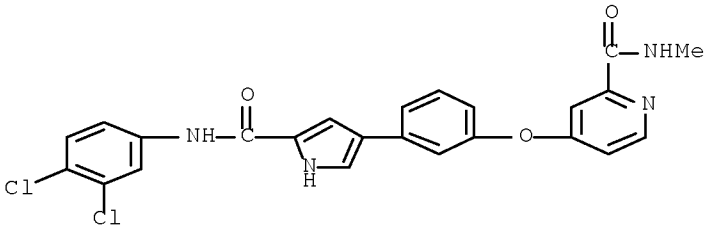
RN 852455-29-9 CAPLUS
CN 2-Pyridinecarboxamide, N-methyl-4-[3-[5-[[[3-(trifluoromethoxy)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]- (CA INDEX NAME)



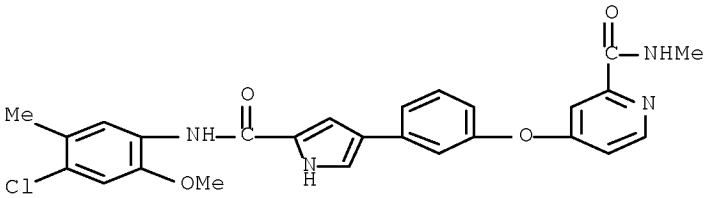
RN 852455-30-2 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



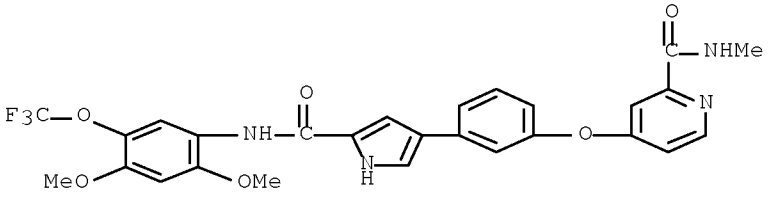
RN 852455-31-3 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[(3,4-dichlorophenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



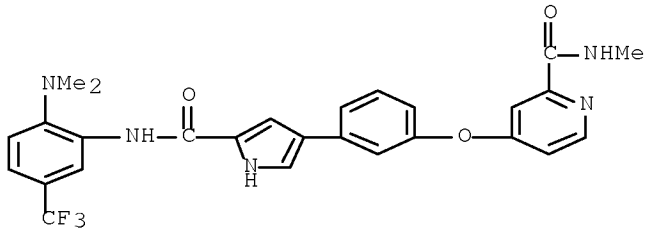
RN 852455-32-4 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[(4-chloro-2-methoxy-5-methylphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



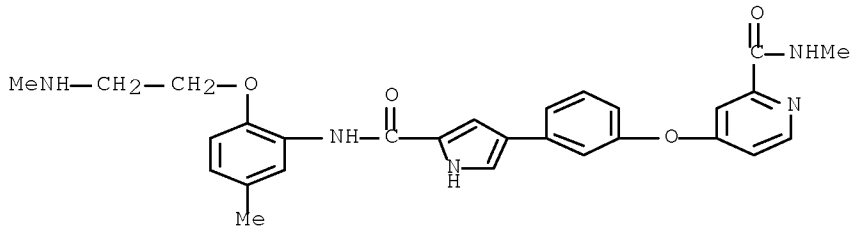
RN 852455-33-5 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2,4-dimethoxy-5-(trifluoromethoxy)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



RN 852455-34-6 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-(dimethylamino)-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



RN 852455-35-7 CAPLUS
CN 2-Pyridinecarboxamide, N-methyl-4-[3-[5-[[[5-methyl-2-[2-(methylamino)ethoxy]phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]- (CA INDEX NAME)



RN 852455-36-8 CAPLUS
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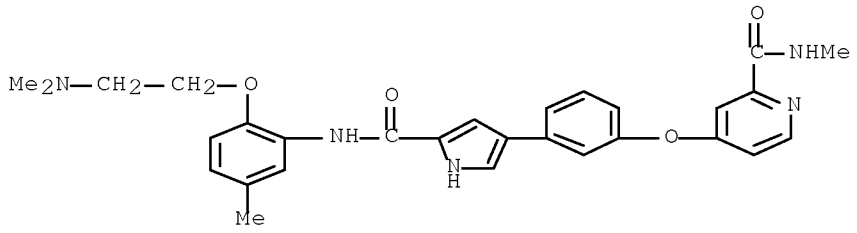
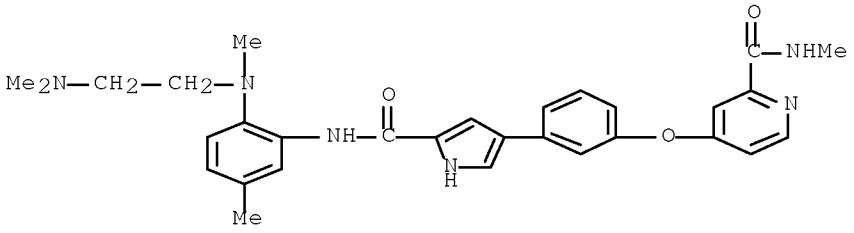


RN 852455-37-9 CAPLUS
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-[[2-(dimethylamino)ethyl]methylamino]-5-methylphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



L3 ANSWER 18 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:570508 CAPLUS Full-text
DOCUMENT NUMBER: 141:106366
TITLE: Preparation of substituted pyrroles as kinase inhibitors
INVENTOR(S): Sun, Connie Li; Tang, Peng Cho; Ockey, Denise
PATENT ASSIGNEE(S): Sugen, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 44 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20040138269	A1	20040715	US 2003-679693		20031007
PRIORITY APPLN. INFO.:			US 2002-417555P	P	20021011

OTHER SOURCE(S): MARPAT 141:106366
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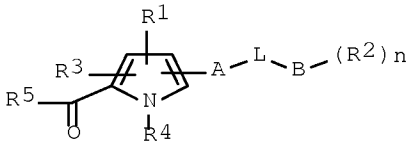

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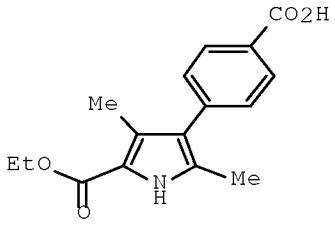


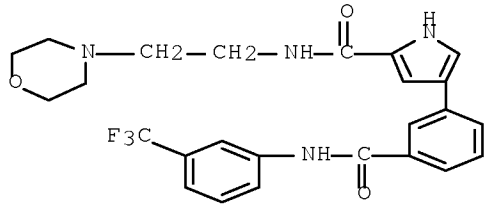
II

AB Title compds. I [R1 = H, alkyl, aryl, heteroaryl; R2 = alkyl, cycloalkyl, aryl, etc.; R3 = H, alkyl; R4 = H, alkyl, cycloalkyl, etc.; R5 = alkyl, cycloalkyl, aryl, heteroaryl, etc.; L = linker, e.g., alkyl-carboxamido, etc.; n = 0-5; A, B = cycloalkyl, aryl, heteroaryl] are prepared For instance, 3,5-dimethyl-1H-pyrrole-2-carboxylic acid Et ester is brominated in the 4-position (CH3CN, NBS, K2CO3) and coupled to 4-carboxyphenylboronic acid (DMF, (PPh3)4Pd, K2CO3, 18 h) to give II. I modulate the activity of protein kinases (PK) and are useful in treating disorders related to abnormal PK activity.

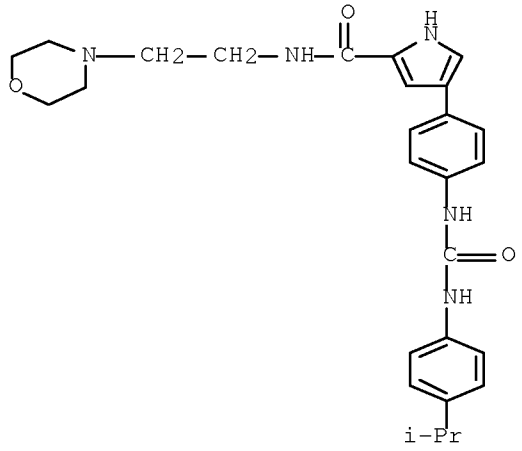
IT 720708-47-4P, 4-[3-(3-Trifluoromethylphenylcarbamoyl)phenyl]-1H-pyrrole-2-carboxylic acid [2-(morpholin-4-yl)ethyl]amide

720708-57-6P, 4-[4-[N'-(4-Isopropylphenyl)ureido]phenyl]-1H-pyrrole-2-carboxylic Acid [2-(morpholin-4-yl)ethyl]amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(substituted pyrroles as kinase inhibitors)

RN 720708-47-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-[2-(4-morpholinyl)ethyl]-4-[3-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]- (CA INDEX NAME)



RN 720708-57-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-[[[4-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)



L3 ANSWER 19 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:292020 CAPLUS Full-text
DOCUMENT NUMBER: 140:321233
TITLE: A preparation of pyrrole derivatives useful for the treatment of disorders ameliorated by reduction of TNF-α production and/or p38 activity
INVENTOR(S): Bullington, James L.; Fan, Xiaodong; Jackson, Paul F.; Zhang, Yue-mei
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 116 pp.

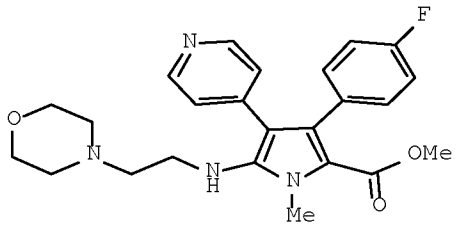
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029040	A1	20040408	WO 2003-US30223	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500221	A1	20040408	CA 2003-2500221	20030924
AU 2003278927	A1	20040419	AU 2003-278927	20030924
US 20050043331	A1	20050224	US 2003-670031	20030924
EP 1549635	A1	20050706	EP 2003-770442	20030924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014783	A	20050726	BR 2003-14783	20030924
CN 1701069	A	20051123	CN 2003-825319	20030924
JP 2006511479	T	20060406	JP 2004-539896	20030924
MX 2005PA03264	A	20051018	MX 2005-PA3264	20050328
NO 2005001967	A	20050621	NO 2005-1967	20050422
ZA 2005003383	A	20060726	ZA 2005-3383	20050426
IN 2005KN00739	A	20060630	IN 2005-KN739	20050427

PRIORITY APPLN. INFO.:			US 2002-414436P	P 20020927
			WO 2003-US30223	W 20030924

OTHER SOURCE(S): MARPAT 140:321233
GI

I



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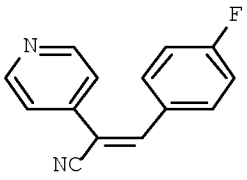
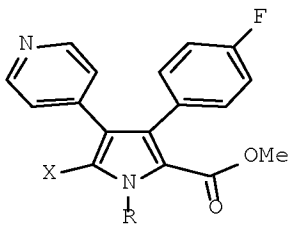


III

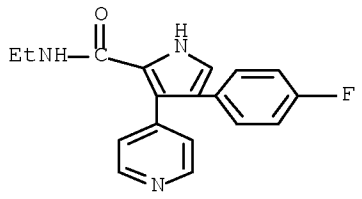


IV

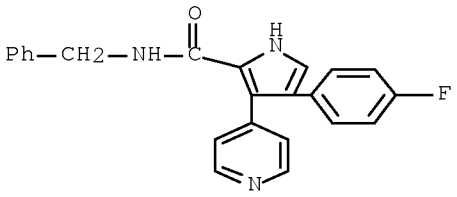
AB The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un)substituted alkyl, (un)substituted (hetero)aryl, etc.; R5 = (un)substituted alkyl, C(O)OR7, C(O)R7, CN, NO2, halo, etc.; R6 and R7 are independently selected from H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF-α production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and TNF-α inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF-α production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanoacetate, N-methylation of the pyrrole ring of the obtained pyrrolecarboxylate derivative IV (X = H, R = H), bromination of the pyrrolecarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.

IT 678161-63-2P 678161-84-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF-α production and/or p38 activity)

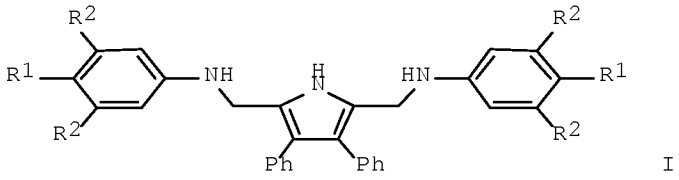
RN 678161-63-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-ethyl-4-(4-fluorophenyl)-3-(4-pyridinyl)- (CA INDEX NAME)



RN 678161-84-7 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-fluorophenyl)-N-(phenylmethyl)-3-(4-pyridinyl)- (CA INDEX NAME)



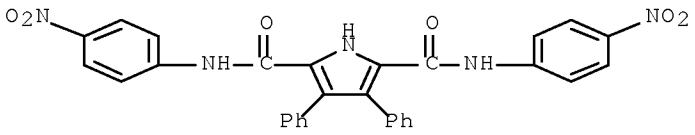
L3 ANSWER 20 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:290714 CAPLUS Full-text
DOCUMENT NUMBER: 139:133415
TITLE: Nitrophenyl derivatives of pyrrole 2,5-diamides: structural behavior, anion binding and color change signaled deprotonation
AUTHOR(S): Camiolo, Salvatore; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Organic & Biomolecular Chemistry (2003), 1(4), 741-744
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133415
GI



I

AB Two new pyrrole 2,5-diamide clefts (I; R1 = NO2, R2 = H; R1 = H, R2 = NO2) have been synthesized. The 3,5-dinitrophenyl derivative has been shown to deprotonate in the presence of fluoride, which in acetonitrile solution, gives rise to a deep blue color.

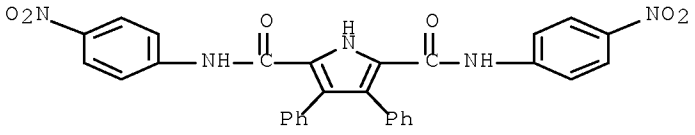
IT 566932-84-1P 566932-86-3P 566932-87-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and x-ray anal. of)
RN 566932-84-1 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(4-nitrophenyl)-3,4-diphenyl- (CA INDEX NAME)



RN 566932-86-3 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N,N'-bis(4-nitrophenyl)-3,4-diphenyl-, compd. with sulfinylbis[methane] (1:3) (9CI) (CA INDEX NAME)

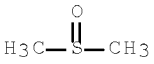
CM 1

CRN 566932-84-1
CMF C30 H21 N5 O6



CM 2

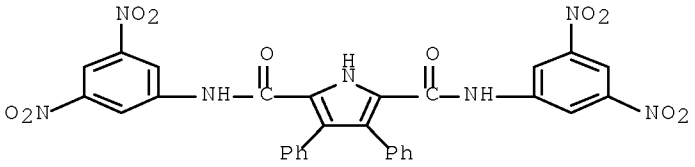
CRN 67-68-5
CMF C2 H6 O S



RN 566932-87-4 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N,N'-bis(3,5-dinitrophenyl)-3,4-diphenyl-, compd. with sulfinylbis[methane] (1:2) (9CI) (CA INDEX NAME)

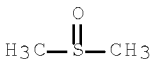
CM 1

CRN 566932-85-2
CMF C30 H19 N7 O10

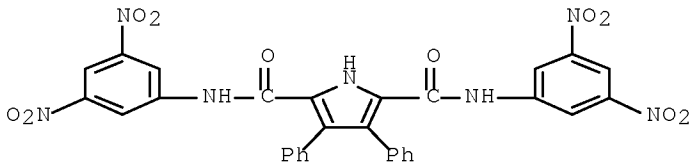


CM 2

CRN 67-68-5
CMF C2 H6 O S



IT 566932-85-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, x-ray anal., and chloride binding of)
RN 566932-85-2 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(3,5-dinitrophenyl)-3,4-diphenyl- (CA INDEX NAME)



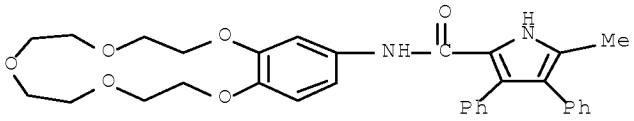
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:276159 CAPLUS Full-text
DOCUMENT NUMBER: 139:350593
TITLE: Crown Ether Appended Amidopyrrole Clefts
AUTHOR(S): Camiolo, Salvatore; Coles, Simon J.; Gale, Philip A.; Hursthouse, Michael B.; Tizzard, Graham J.
CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Supramolecular Chemistry (2003), 15(3), 231-234
CODEN: SCHEER; ISSN: 1061-0278
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:350593
AB Two new pyrrole amide-crown ether conjugates have been synthesized and their anion complexation properties studied in the absence and presence of stoichiometric quantities of sodium or cesium cations. Certain anions are sequestered by the metal cation in DMSO-d6 (0.5% water), however, in one case a 4.7 fold increase in the fluoride affinity of the receptor was observed upon addition of caesium cations. Crystal structure of one of the products was also reported.
IT 619328-75-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation and crystal structure of crown ether-appended amidopyrrole clefts and their anion complexation in presence of sodium or cesium cations)

RN 619328-75-5 CAPLUS

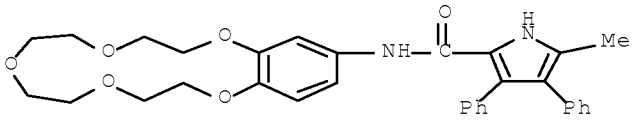
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX NAME)



IT 619328-75-5DP, halide, benzoate, and phosphate complexes
619328-76-6DP, halide, benzoate, and phosphate complexes
619328-76-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of crown ether-appended amidopyrrole clefts and their anion complexation in presence of sodium or cesium cations)

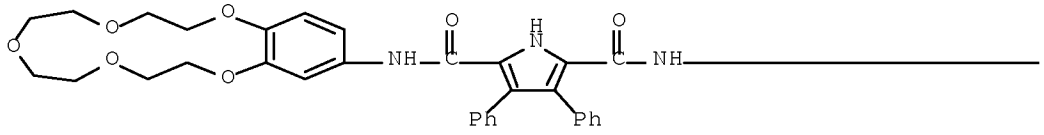
RN 619328-75-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX NAME)

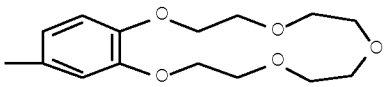


RN 619328-76-6 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX NAME)

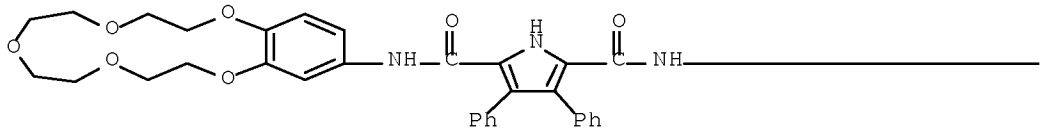


PAGE 1-B

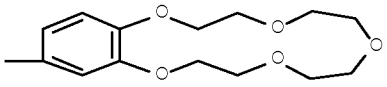


RN 619328-76-6 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX NAME)

PAGE 1-A

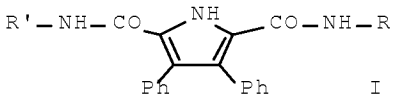


PAGE 1-B



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:126247 CAPLUS Full-text
DOCUMENT NUMBER: 139:133642
TITLE: Mono- and bis-ferrocene 2,5-diamidopyrrole clefts: solid-state assembly, anion binding and electrochemical properties
AUTHOR(S): Coles, Simon J.; Denuault, Guy; Gale, Philip A.; Horton, Peter N.; Hursthouse, Michael B.; Light, Mark E.; Warriner, Colin N.
CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Polyhedron (2003), 22(5), 699-709
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133642
GI



I

AB Four amido-pyrrole cleft anion receptors bearing one or two ferrocene reporter groups, e.g., I [R = R' = CH2Fc 1, Fc 2; R = Ph, R' = CH2Fc 3, Fc 4, Fc = (C5H5)2Fe] were synthesized and crystallog. characterized. The receptors contain either a nonconjugated (1 and 3) or conjugated (2 and 4) link between the anion binding amido-pyrrole unit and the ferrocene reporter groups. The anion binding affinities and electrochem. behavior of the receptors in the absence and presence of anions were studied by 1H NMR titration techniques and cyclic voltammetry using a Pt microdisc working electrode, resp.

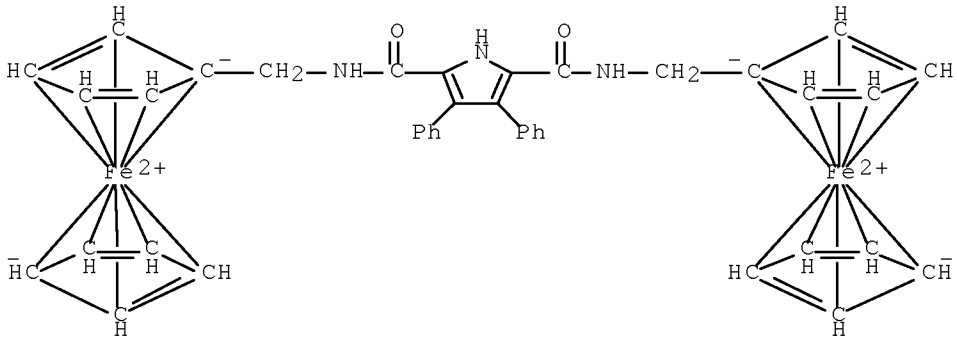
IT 475148-10-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(crystal structure, electrochem.; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

RN 475148-10-8 CAPLUS

CN Ferrocene, 1,1''-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonyliminomethylene)]bis- (9CI) (CA INDEX NAME)



IT 566915-30-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)

RN 566915-30-8 CAPLUS

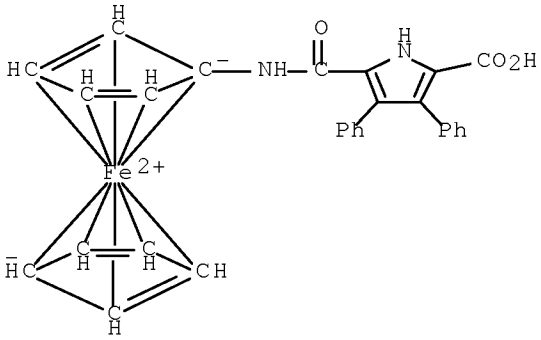
CN Ferrocene, [[(5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl)carbonyl]amino]-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 566915-29-5

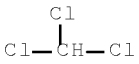
CMF C28 H22 Fe N2 O3

CCI CCS

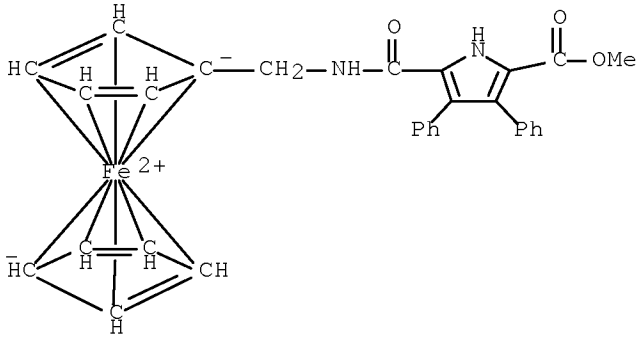


CM 2

CRN 67-66-3
CMF C H Cl3

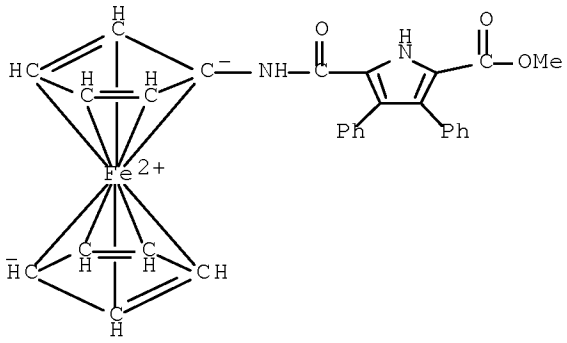


IT 566915-24-0P 566915-25-1P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure; preparation and saponification in the synthesis of mono- and
bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)
RN 566915-24-0 CAPLUS
CN Ferrocene, [[[[5-(methoxycarbonyl)-3,4-diphenyl-1H-pyrrol-2-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



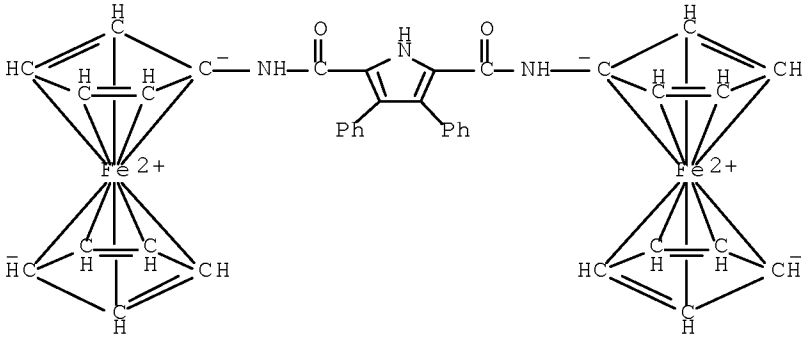
RN 566915-25-1 CAPLUS
CN Ferrocene, [[[5-(methoxycarbonyl)-3,4-diphenyl-1H-pyrrol-2-

yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

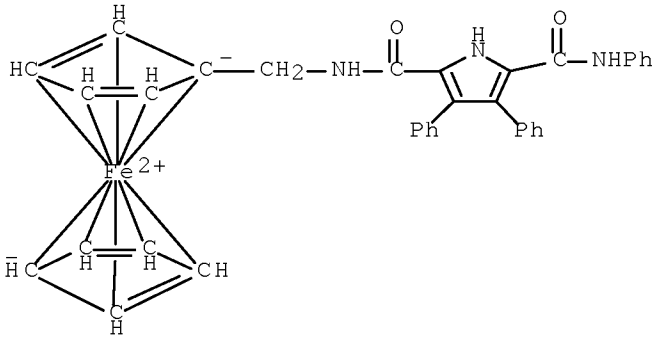


IT 475148-12-0P 566915-20-6P 566915-22-8P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystal structure; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

RN 475148-12-0 CAPLUS
CN Ferrocene, 1,1''-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis- (9CI) (CA INDEX NAME)



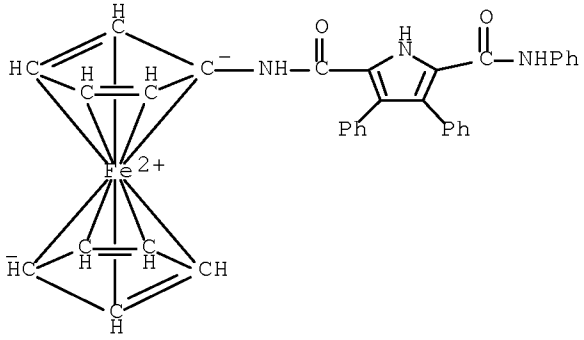
RN 566915-20-6 CAPLUS
CN Ferrocene, [[[[3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 566915-22-8 CAPLUS
CN Ferrocene, [[[3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]-, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 566915-21-7
CMF C34 H27 Fe N3 O2
CCI CCS



CM 2

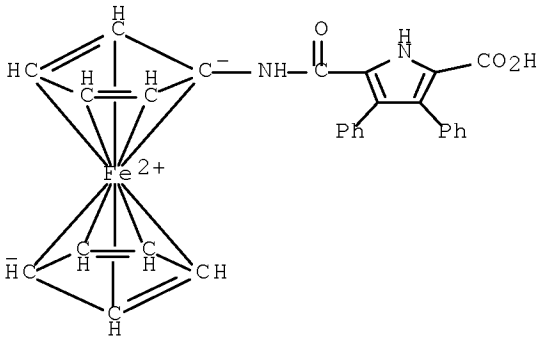
CRN 67-56-1
CMF C H4 O

IT 566915-29-5P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mol. structure; preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion

receptors)

RN 566915-29-5 CAPLUS

CN Ferrocene, [[(5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)



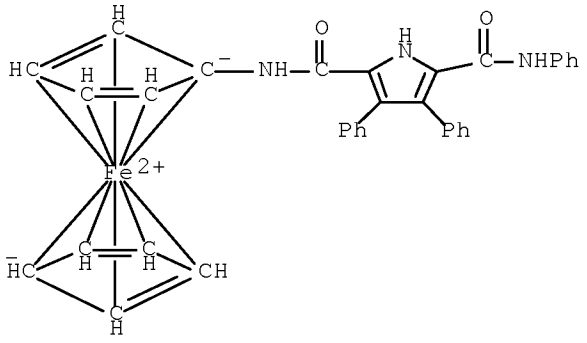
IT 566915-21-7P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(mol. structure; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

RN 566915-21-7 CAPLUS

CN Ferrocene, [[[3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



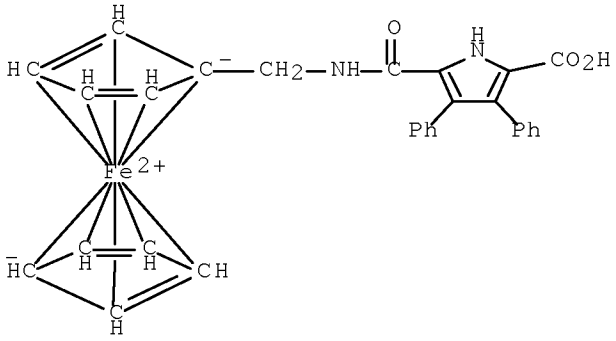
IT 566915-26-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)

RN 566915-26-2 CAPLUS

CN Ferrocene, [[[(5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl)carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

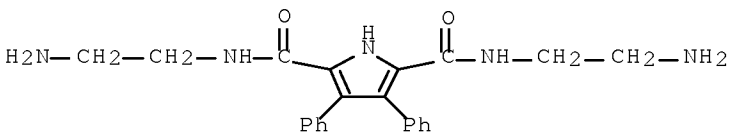
L3 ANSWER 23 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:689617 CAPLUS Full-text
DOCUMENT NUMBER: 138:62059
TITLE: Pendant arm pyrrolic amide cleft anion receptors
AUTHOR(S): Navakhun, Korakot; Gale, Philip A.; Camiolo, Salvatore; Light, Mark E.; Hursthouse, Michael B.
CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (18), 2084-2085
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The propensity of amine, ammonium and amide pendant arm 2,5-diamidopyrrole derivs. to act as anion receptors has been investigated. The anion-coordination ability of these species has been determined by 1H NMR titration techniques revealing a marked selectivity of the amine functionalized receptor for hydrogen sulfate anions.

IT 479401-36-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(X-ray structure of pendant arm pyrrolic amide cleft receptors)
RN 479401-36-0 CAPLUS
CN Phosphate(1-), hexafluoro-, hydrogen, compd. with N,N'-bis(2-aminoethyl)-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (1:1), dihydrate (9CI) (CA INDEX NAME)

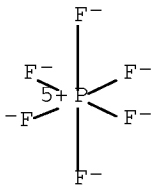
CM 1

CRN 479401-33-7
CMF C22 H25 N5 O2



CM 2

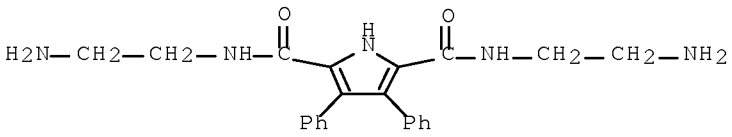
CRN 16940-81-1
CMF F6 P . H
CCI CCS



IT 479401-34-8P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(pendant arm pyrrolic amide cleft anion receptors)
RN 479401-34-8 CAPLUS
CN Phosphate(1-), hexafluoro-, hydrogen, compd. with N,N'-bis(2-aminoethyl)-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (2:1) (9CI) (CA INDEX NAME)

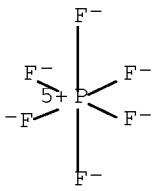
CM 1

CRN 479401-33-7
CMF C22 H25 N5 O2

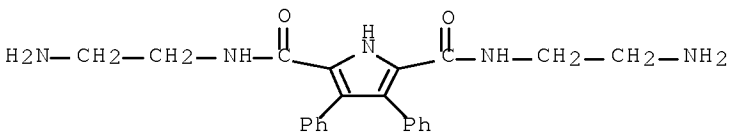


CM 2

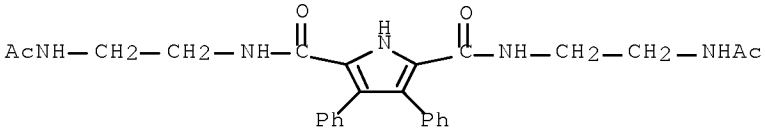
CRN 16940-81-1
CMF F6 P . H
CCI CCS



IT 479401-33-7P 479401-35-9P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(pendant arm pyrrolic amide cleft anion receptors)
RN 479401-33-7 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(2-aminoethyl)-3,4-diphenyl- (CA INDEX NAME)



RN 479401-35-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis[2-(acetylamino)ethyl]-3,4-diphenyl- (CA INDEX NAME)



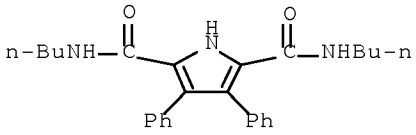
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:675089 CAPLUS Full-text
DOCUMENT NUMBER: 138:122276
TITLE: Confirmation of a cleft-mode' of binding in a 2,5-diamidopyrrole anion receptor in the solid state
AUTHOR(S): Camiolo, Salvatore; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.
CORPORATE SOURCE: University of Southampton, Department of Chemistry, Southampton, SO17 1BJ, UK
SOURCE: Tetrahedron Letters (2002), 43(39), 6995-6996

CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystal structure of the tetrabutylammonium benzoate complex of 3,4-diphenyl-1H-pyrrole-2,5-dicarboxylic acid bis-butylamide has been elucidated confirming the formation of a cleft conformation in the solid state upon anion binding.
IT 488787-58-2
RL: PRP (Properties)
(crystal structure; crystal structure of tetrabutylammonium benzoate complex of diphenylpyrroledicarboxylic acid bis-butylamide)
RN 488787-58-2 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, benzoate, compd. with N,N'-dibutyl-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 365214-49-9
CMF C26 H31 N3 O2

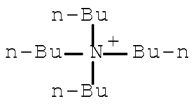


CM 2

CRN 18819-89-1
CMF C16 H36 N . C7 H5 O2

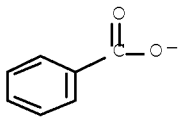
CM 3

CRN 10549-76-5
CMF C16 H36 N



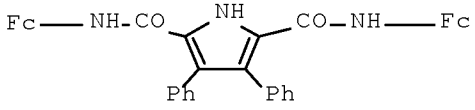
CM 4

CRN 766-76-7
CMF C7 H5 O2

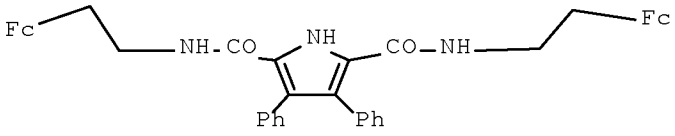


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:477989 CAPLUS Full-text
DOCUMENT NUMBER: 137:370181
TITLE: Anion complexation and electrochemical behavior of ferrocene-appended amido-pyrrole clefts
AUTHOR(S): Denuault, Guy; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.; Warriner, Colin N.
CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: New Journal of Chemistry (2002), 26(7), 811-813
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:370181
GI



I



II

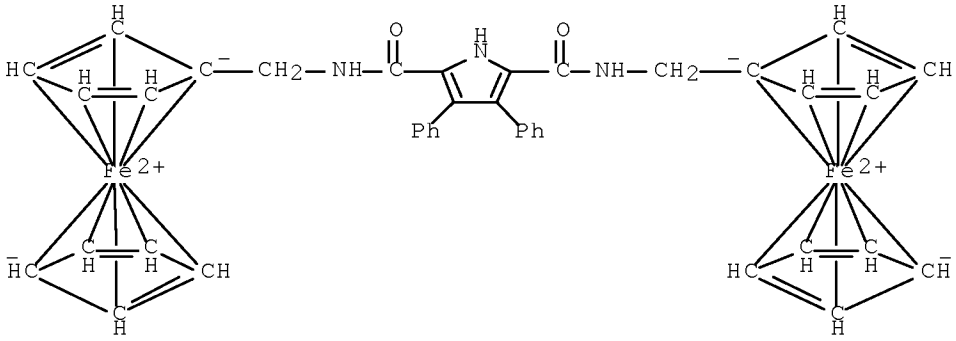
AB Two amido-pyrrole cleft anion receptors bearing two ferrocene reporter groups, e.g., I and II [Fc = (C5H4)Fe(C5H5)] were synthesized and crystallog. characterized; the receptors contain either a nonconjugated or conjugated link between the anion-binding amido-pyrrole unit and the ferrocene reporter groups. The anion binding affinities and electrochem. behavior of the receptors in the absence and presence of anions were studied by 1H NMR titration techniques and cyclic voltammetry using a Pt microdisc working electrode, resp.

IT 475148-10-8P 475148-12-0P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical

process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, electrochem. and crystal structure of)

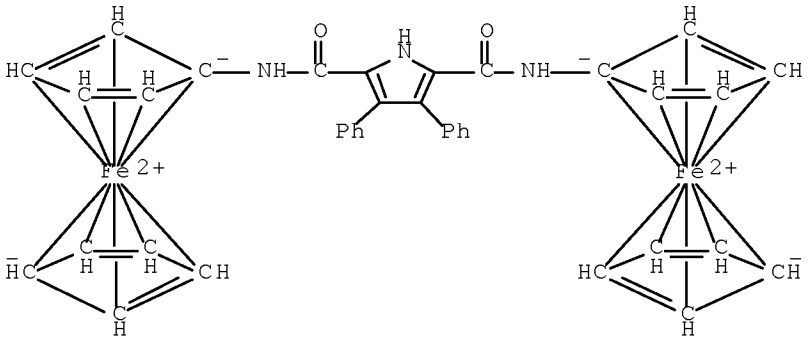
RN 475148-10-8 CAPLUS

CN Ferrocene, 1,1''-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonyliminomethylene)]bis- (9CI) (CA INDEX NAME)



RN 475148-12-0 CAPLUS

CN Ferrocene, 1,1''-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 26 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:219745 CAPLUS Full-text

DOCUMENT NUMBER: 137:109012

TITLE: Solution and solid-state studies of 3,4-dichloro-2,5-diamidopyrroles: formation of an unusual anionic narcissistic dimer

AUTHOR(S): Camiolo, Salvatore; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.; Shi, Andy J.

CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

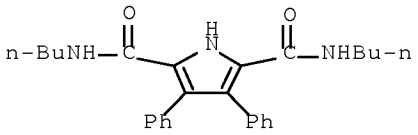
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (7), 758-759

CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:109012

AB 3,4-Dichoro-1H-pyrrole-2,5-dicarboxylic acid bis-phenylamide 3 and 3,4-dichloro-1H-pyrrole-2,5-dicarboxylic acid bis-butylamide 4 were prepared and shown to deprotonate in the presence of basic anions: the x-ray crystal structure of the tetrabutylammonium salt of 3-H+ reveals the formation of a dimer in the solid state.

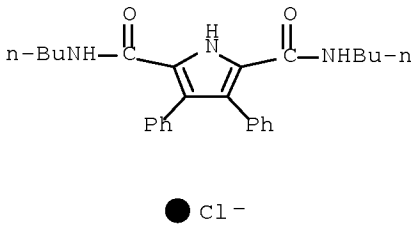
IT 365214-49-9
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(chloride receptor; solution and solid-state studies of unusual anionic narcissistic dimer of 3,4-dichloro-2,5-diamidopyrroles)

RN 365214-49-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



IT 443785-00-0
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(solution and solid-state studies of unusual anionic narcissistic dimer of 3,4-dichloro-2,5-diamidopyrroles)

RN 443785-00-0 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

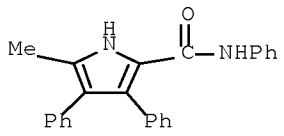
L3 ANSWER 27 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:759709 CAPLUS Full-text
DOCUMENT NUMBER: 136:37467
TITLE: 2-Amidopyrroles and 2,5-Diamidopyrroles as Simple Anion Binding Agents
AUTHOR(S): Gale, Philip A.; Camiolo, Salvatore; Tizzard, Graham J.; Chapman, Christopher P.; Light, Mark E.; Coles,

Simon J.; Hursthouse, Michael B.
CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Journal of Organic Chemistry (2001), 66(23), 7849-7853
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:37467
AB Four new 2-pyrrolecarboxamides and 2,5-pyrroledicarboxamides have been synthesized and their anion complexation properties investigated. The crystal structures of these receptors have been elucidated and reveal hydrogen bonding in the solid state leading to dimer and network formation. Selectivity for oxo-anions has been demonstrated by 1H NMR titration techniques; the 2,5-pyrroledicarboxamides are particularly selective for dihydrogen phosphate and benzoate over halide anions.
IT 380537-10-0 380537-11-1
RL: PRP (Properties)
(crystal structure; preparation, crystal structures, and anion complexation properties of pyrrolecarboxamides and pyrroledicarboxamides)

RN 380537-10-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N,3,4-triphenyl-, compd. with dichloromethane (2:1) (9CI) (CA INDEX NAME)

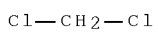
CM 1

CRN 380537-09-7
CMF C24 H20 N2 O



CM 2

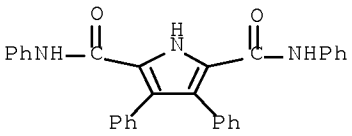
CRN 75-09-2
CMF C H2 Cl2



RN 380537-11-1 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N,N',3,4-tetraphenyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

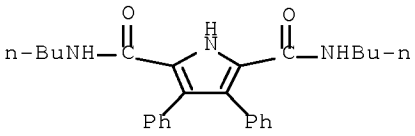
CRN 365214-50-2
CMF C30 H23 N3 O2



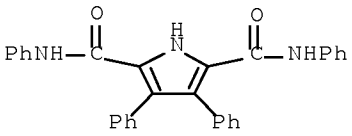
CM 2

CRN 67-68-5
CMF C2 H6 O S

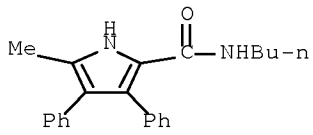
IT 365214-49-9P 365214-50-2P 380537-08-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation, crystal structures, and anion complexation properties of pyrrolecarboxamides and pyrroledicarboxamides)
RN 365214-49-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



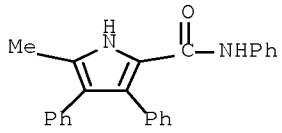
RN 365214-50-2 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



RN 380537-08-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-butyl-5-methyl-3,4-diphenyl- (CA INDEX NAME)

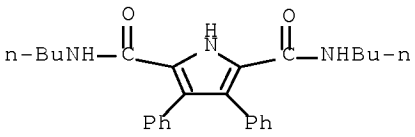


IT 380537-09-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structures, and anion complexation properties of pyrrolecarboxamides and pyrroledicarboxamides)
RN 380537-09-7 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N,3,4-triphenyl- (CA INDEX NAME)

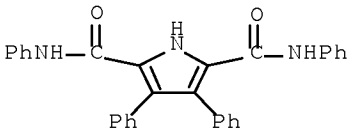


REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 28 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:498916 CAPLUS Full-text
DOCUMENT NUMBER: 135:288487
TITLE: Hydrogen-bonding pyrrolic amide cleft anion receptors
AUTHOR(S): Gale, P. A.; Camiolo, S.; Chapman, C. P.; Light, M. E.; Hursthouse, M. B.
CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
SOURCE: Tetrahedron Letters (2001), 42(30), 5095-5097
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:288487
AB The use of simple 2,5-diamidopyrrole derivs. as anion receptors has been investigated. Reaction of 3,4-diphenylpyrrole-2,5-dicarboxylic acid chloride with n-butylamine or aniline has produced two new amidic cleft anion receptors 1 and 2. The anion-coordination ability of these species has been determined by 1H NMR titration techniques. Crystal structures of 1 and 2 have been elucidated, revealing a continuous hydrogen bonding network formed by 1 and dimerization of 2 via NH···O and CH···O hydrogen bonds.
IT 365214-49-9 365214-50-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(anion receptor; hydrogen-bonding pyrrolic amide cleft anion receptors)
RN 365214-49-9 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)

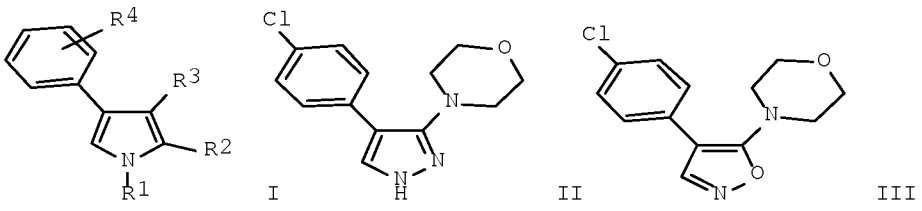


RN 365214-50-2 CAPLUS
CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 29 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:115 CAPLUS Full-text
DOCUMENT NUMBER: 128:84047
ORIGINAL REFERENCE NO.: 128:16249a,16252a
TITLE: Synthesis, Anticonvulsant Activity, and Structure-Activity Relationships of Sodium Channel Blocking 3-Aminopyrroles
AUTHOR(S): Unverferth, Klaus; Engel, Juergen; Hoefgen, Norbert; Rostock, Angelika; Guenther, Ralf; Lankau, Hans-Joachim; Menzer, Manfred; Rolfs, Andreas; Liebscher, Juergen; Mueller, Birgit; Hofmann, Hans-Joerg
CORPORATE SOURCE: Corporate Research and Development ASTA Medica Group, Arzneimittelwerk Dresden GmbH, Radebeul, D-01445, Germany
SOURCE: Journal of Medicinal Chemistry (1998), 41(1), 63-73
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

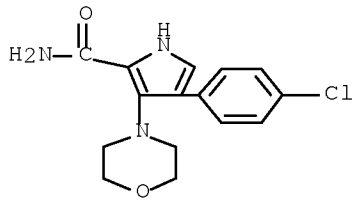


I II III

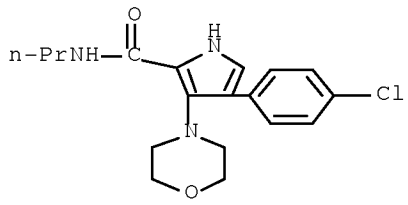
AB Starting from the corresponding acetophenone and glycine derivs., a series of new 3-aminopyrroles I [R1 = H, Me, PhCH2, Ac, PrCO, Bz, PhO2C, 4-morpholinylcarbonyl, EtSO2; R2 = CO2Me, CO2Et, CN, CO2CH2CHMe2, CO2H, H, CONH2, CONHPr, CONHCH2CH:CH2, CONHCH2CH2OMe, CONMe2, 4-morpholinylcarbonyl, 1-(4-methylpiperazinyl)carbonyl, COMe, CH2CH2CO2Me; R3 = 4-morpholinyl, NEt2, NMe2, 4-phenyl-1-piperazinyl, 4-methyl-1-piperazinyl, NMeCH2CH2NMe2; R4 = 4-Cl, 4-Br, 3-Br, 2-Me, H, 4-F, 4-Et] was synthesized in few steps. Using this procedure with hydrazine and hydroxylamine instead of the glycinates provides access to 3-aminopyrazole II and 5-amino-1,2-oxazole III. The various derivs. were tested for anticonvulsant activity in a variety of test models. Several compds. exhibit considerable activity with a remarkable lack of neurotoxicity. Ester I (R1 = H, R2 = CO2Me, R3 = 4-morpholinyl, R4 = 4-Br) (IV) was the most active compound IV was protective in the maximal electroshock seizure (MES) test in rats with an oral ED50 of 2.5 mg/kg with no neurotoxicity noted at doses up to 500 mg/kg. IV blocks sodium channels in a frequency-dependent manner. The essential structural features which could be responsible for an interaction with an active site of the voltage-dependent sodium channel are established within a suggested pharmacophore model.

IT 183591-88-0P 200862-96-0P 200862-97-1P 200862-98-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, anticonvulsant activity, and structure-activity relationships of sodium channel blocking aminopyrroles)

RN 183591-88-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX NAME)

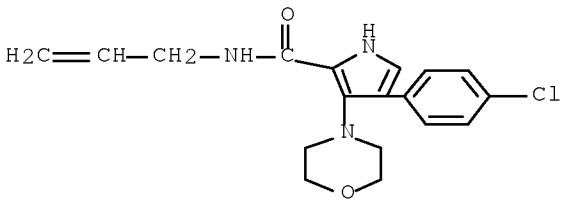


RN 200862-96-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)-N-propyl- (CA INDEX NAME)

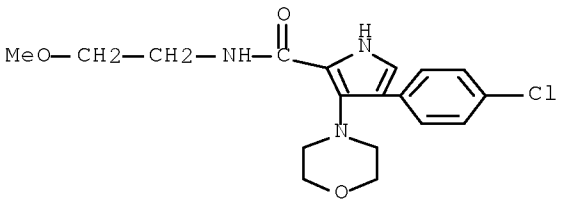


RN 200862-97-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)-N-2-propen-1-yl- (CA INDEX NAME)



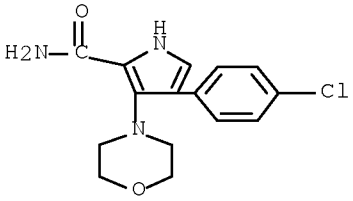
RN 200862-98-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-(2-methoxyethyl)-3-(4-morpholinyl)- (CA INDEX NAME)



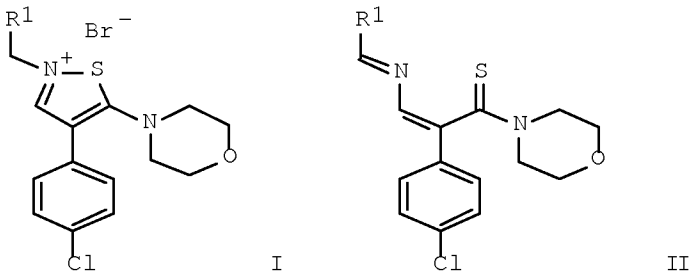
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 30 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:120169 CAPLUS Full-text
DOCUMENT NUMBER: 126:199420
ORIGINAL REFERENCE NO.: 126:38551a,38554a
TITLE: Mechanistic aspects of the synthesis of 3-aminopyrroles from substituted 2-methyl-1,2-thiazolium salts or 3-aminothioacrylamides. [Erratum to document cited in CA126:7936]
AUTHOR(S): Rolfs, Andreas; Jones, Peter G.; Liebscher, Juergen
CORPORATE SOURCE: Inst. Chemie, Humboldt-Univ., Berlin, D-10115, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (2), 183
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In Scheme 2, the structure for compound 6 is corrected The error was not reflected in the abstract or the index entries.
IT 183591-88-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroles by ring transformation and desulfurization of thiazolium compds. (Erratum))
RN 183591-88-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX

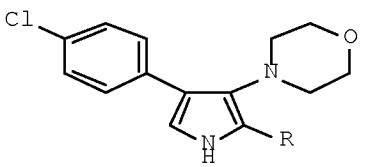
NAME)



L3 ANSWER 31 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:635701 CAPLUS Full-text
DOCUMENT NUMBER: 126:7936
ORIGINAL REFERENCE NO.: 126:1767a,1770a
TITLE: Mechanistic aspects of the synthesis of 3-aminopyrroles from substituted 2-methyl-1,2-thiazolium salts or 3-aminothioacrylamides
AUTHOR(S): Rolfs, Andreas; Jones, Peter G.; Liebscher, Juergen
CORPORATE SOURCE: Inst. Chemie, Humboldt-Univ., Berlin, D-10115, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1996), (19), 2339-2343
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:7936
GI



I II



III

AB The mechanism of the synthesis of 3-aminopyrrole derivs. by ring transformation-desulfurization of substituted 2-methyl-1,2-thiazolium salts

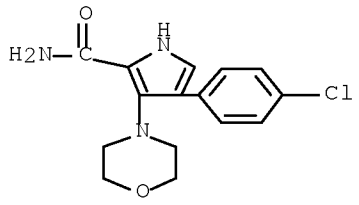
was investigated. The thiazolium salts I (R1 = 4-nitrophenyl, amido) were transformed into the thioamide derivs. II (same R1). II were subsequently transformed into the pyrroles III (R = cyano, amido).

IT 183591-88-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroles by ring transformation and desulfurization of thiazolium compds.)

RN 183591-88-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX NAME)



L3 ANSWER 32 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:994741 CAPLUS Full-text

DOCUMENT NUMBER: 124:86809

ORIGINAL REFERENCE NO.: 124:16315a,16318a

TITLE: Preparation of (pyrrolyl- and thienylcarbonyl)guanidines as sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell proliferation inhibitors

INVENTOR(S): Kleemann, Heinz-Werner; Lang, Hans-Jochen; Schwark, Jan-Robert; Weichert, Andreas; Scholz, Wolfgang; Albus, Udo

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

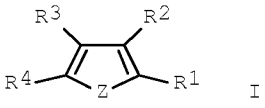
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 676395	A2	19951011	EP 1995-105088	19950405
EP 676395	A3	19960306		
EP 676395	B1	20030903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
DE 4412334	A1	19951019	DE 1994-4412334	19940411
AT 248817	T	20030915	AT 1995-105088	19950405
ES 2206471	T3	20040516	ES 1995-105088	19950405
FI 9501681	A	19951012	FI 1995-1681	19950407
AU 9516354	A	19951019	AU 1995-16354	19950407
AU 683722	B2	19971120		
US 5698581	A	19971216	US 1995-418434	19950407
CA 2146707	A1	19951012	CA 1995-2146707	19950410
CA 2146707	C	20081021		
NO 9501405	A	19951012	NO 1995-1405	19950410

JP 07291927	A	19951107	JP 1995-107811		19950410
JP 4171078	B2	20081022			
ZA 9502930	A	19960126	ZA 1995-2930		19950410
HU 71616	A2	19960129	HU 1995-1035		19950410
CN 1117044	A	19960221	CN 1995-104391		19950410
CN 1073988	C	20011031			
IL 113310	A	20000629	IL 1995-113310		19950410
PRIORITY APPLN. INFO.:			DE 1994-4412334	A	19940411

OTHER SOURCE(S): MARPAT 124:86809

GI



I

AB Title compds. [I; 1 of R1,R2 = CON:C(NH2)2 and the other = H, halo, alkyl, CON:C(NH2)2, NH2, etc.; R3,R4 = H, halo, cyano, alkyl, Ph, heteroaryl, etc.; Z = SO0-2, O, NR5; R5 = H, alkyl, etc.] were prepared Thus, Me 1-methylpyrrole-2-carboxylate was alkylated with (CF3)2CFI and the product amidated with guanidine to give I [R1 = CON:C(NH2)2, R2 = R3 = H, R4 = (CF3)2CF, Z = NMe] which ad IC50 of 0.3μM against Na+/H+ exchange in rabbit erythrocytes in vitro.

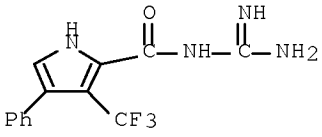
IT 172460-15-0P 172460-16-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (pyrrolyl- and thienylcarbonyl)guanidines as sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell proliferation inhibitors)

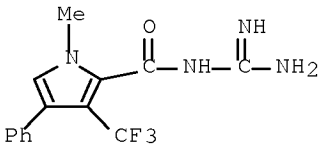
RN 172460-15-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(aminoiminomethyl)-4-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 172460-16-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(aminoiminomethyl)-1-methyl-4-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)



L3 ANSWER 33 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:218959 CAPLUS Full-text
DOCUMENT NUMBER: 122:133846
ORIGINAL REFERENCE NO.: 122:24979a,24982a
TITLE: Preparation of small peptide anaphylatoxin receptor ligands
INVENTOR(S): Or, Yat Sun; Luly, Jay R.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

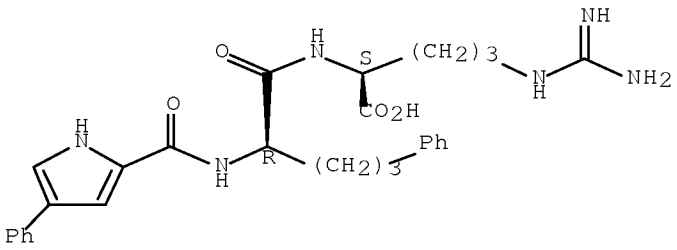
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9407815	A2	19940414	WO 1993-US8173	19930830

W: CA, JP
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRIORITY APPLN. INFO.: US 1992-951684 A 19920925
OTHER SOURCE(S): MARPAT 122:133846

AB Oligopeptide compds. or analogs represented by the formula A-B-D [A = R1-R2; B = R3-R4-R5; D = R6-R7-R8; R1 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, arylalkenyl, arylhydrazino, arylalkylamino, aminoalkyl, heterocyclyl, heterocyclylalkyl; R2 = CO, CS, CH2, SO2; provided that when R2 is CS or SO2, R1 may be H; R3, R6 = NR101 (wherein R101 = H, alkyl, arylalkyl); R4 = CR200R201, NR101, (E)- or (Z)-C:CHR205 (wherein R205 = arylalkyl); R5 = CO, CH2, CH2CO; R7 = CR210R211; R8 = H, CH2CO2H, CO2R100 (R100 = H, alkyl, arylalkyl); R200, R210 = H, alkyl, arylalkyl; R201 = (CH2)3Z (wherein Z = aryl or heterocyclyl attached to (CH2)3 through the ring C atom), CH2XCH2Z (wherein X = O, S, NH, alkylimino; Z = Z = aryl or heterocyclyl attached to CH2XCH2 through the ring C atom), CH2SCHR300W (wherein W = aryl; R300 = CO2H, alkoxycarbonyl, alkyl), CH2CH2XW (X, W = same as above), etc.; R211 = guanidinoalkyl; or R1R2 = H, alkyl, arylalkyl, aminoalkyl, guanidinoalkyl, provided that R1R2 is a group other than arylalkyl, R101 = arylalkyl; R1-R2-R3 = Q (wherein R' = H, alkyl); R1-R2-R3-R4 = arylalkylamino, heterocyclyl, arylalkyl, NHR50NR51 (wherein R50 = aroyl; R51 = aryl, arylalkyl)] are prepared These oligopeptides are ligands for the anaphylatoxin receptor and are useful for modulating C5a anaphylatoxin activity and in the treatment of inflammatory disease states. Thus, R-Arg(Tos)-Merrifield resin (I; R = Boc) was deprotected with 45% CF3CO2H in CH2Cl2 containing anisole and coupled with N-tert-butoxylcarbonyl-(R)-2-amino-5-phenylpentanoic acid by using diisopropylcarbodiimide in CH2Cl2 and DMF to give I [R = (R)-2-amino-5-phenylpentanoyl] which was treated with HF(l) and anisole at 0° for 60 min to give N-[(R)-2-amino-5-phenylpentanoyl]-L-arginine. N-[(R)-2-(2-indolecarbonylamino)-5-phenylpentanoyl]-L-arginine inhibited the binding of 125I-labeled C5a anaphylatoxin to purified PMNL membrane fragments with Ki of 0.56 μM.

IT 159320-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anaphylatoxin receptor ligand and antiinflammatory agent)
RN 159320-93-1 CAPLUS
CN L-Arginine, N2-[5-phenyl-N-[(4-phenyl-1H-pyrrol-2-yl)carbonyl]-D-norvalyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

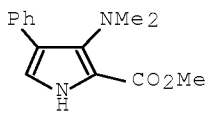


L3 ANSWER 34 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:511467 CAPLUS Full-text
DOCUMENT NUMBER: 117:111467
ORIGINAL REFERENCE NO.: 117:19447a,19450a
TITLE: Preparation of 3-aminopyrroles as analgesics and anticonvulsants
INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter
PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Ger. (East), 6 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298915	A5	19920319	DD 1989-338226	19891117

PRIORITY APPLN. INFO.: DD 1989-338226 19891117
OTHER SOURCE(S): MARPAT 117:111467
GI

I



II

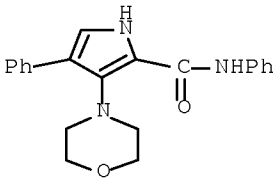
AB Title compds. [I; R = NR3R4; R1 = H, (cyclo)alkyl, arylalkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxycarbonyl, CONH2, (hetero)aryl, cyano, NO2,

etc.; R3, R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; R5R6 = alkylene] were prepared Thus, MeO2CCH2NHCH:CPhC(SMe):N+Me2 I- was cyclized to give title compound II which had ED50 of 4.5 + 10-5 mol/kg orally against maximal electroshock-induced convulsions in mice.

IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic and anticonvulsant)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 35 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:490133 CAPLUS Full-text

DOCUMENT NUMBER: 117:90133

ORIGINAL REFERENCE NO.: 117:15733a,15736a

TITLE: Preparation aminopyrroles as analgesics and anticonvulsants

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany

SOURCE: Ger. (East), 7 pp.
CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

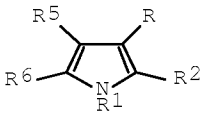
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298914	A5	19920319	DD 1989-338219	19891117

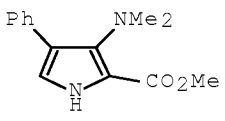
PRIORITY APPLN. INFO.: DD 1989-338219 19891117

OTHER SOURCE(S): MARPAT 117:90133

GI



I



II

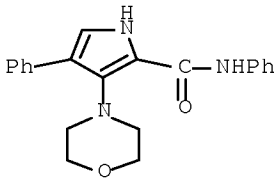
AB The compds. [I; R = NR3R4; R1 = H, (cyclo)alkyl, aralkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxycarbonyl, CONH2, (hetero)aryl, cyano, NO2, etc.; R3,

R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; or NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene] were prepared Thus Me2NCH:CHCSNMe2 was cyclocondensed with H2NCH2CO2Me to give title compound II which had ED50 of 4.5 + 10-5 mol/kg p.o. for protection of mice against maximal electroshock-induced convulsions.

IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, an analgesic and anticonvulsant)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 36 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:490132 CAPLUS Full-text

DOCUMENT NUMBER: 117:90132

ORIGINAL REFERENCE NO.: 117:15733a,15736a

TITLE: Preparation of 3-aminopyrroles as anticonvulsants and analgesics

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany

SOURCE: Ger. (East), 5 pp.
CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

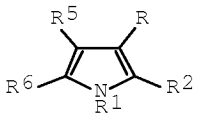
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298918	A5	19920319	DD 1989-340208	19891117

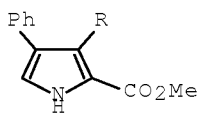
PRIORITY APPLN. INFO.: DD 1989-340208 19891117

OTHER SOURCE(S): CASREACT 117:90132; MARPAT 117:90132

GI



I

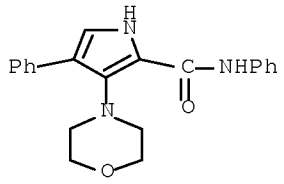


II

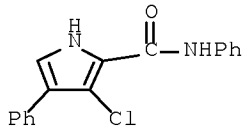
AB Title compds. [I; R = NR3R4; R1 = H, (cyclo)alkyl, aralkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxycarbonyl, CONH2 (hetero)aryl cyano, NO2, etc.;

R3,R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; R5R6 = alkylene] were prepared Thus, pyrrole II (R = SH) was condensed with HNMe2 to give II (R = NMe2) which had ED50 of 4.5 + 10-5 mol/kg orally for protection of mice against maximal electroshock-induced convulsions.

IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic and anticonvulsant)
RN 135548-47-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



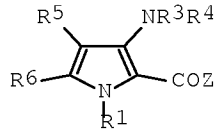
IT 142641-86-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of analgesics and anticonvulsants)
RN 142641-86-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-chloro-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 37 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:469726 CAPLUS Full-text
DOCUMENT NUMBER: 117:69726
ORIGINAL REFERENCE NO.: 117:12263a,12266a
TITLE: Process for preparation of 3-aminopyrrolecarboxylic acid derivatives as anticonvulsants and analgesics
INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter
PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Ger. (East), 6 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298916	A5	19920319	DD 1989-340206	19891117

PRIORITY APPLN. INFO.: DD 1989-340206 19891117
OTHER SOURCE(S): MARPAT 117:69726
GI

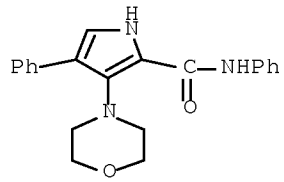


I

AB Nineteen title compds. I [R1 = H, (un)substituted alkyl, (un)substituted cycloalkyl, aralkyl, (un)substituted (hetero)aryl, acyl, alkoxycarbonyl, (un)substituted amino(thio)carbonyl; Z = OH, O-Metal, alkoxy, aryloxy, (un)substituted amino, alkylthio, arylthio; R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted (hetero)aryl; R4 = (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted (hetero)aryl; or R3R4 = alkylene optionally containing O, S, or N as a ring atom; R5 = (un)substituted (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene] were prepared by standard functional transformations of the carboxylic acid moiety or its derived groups. For example, I [R1 = R6 = H, Z = OMe, R3R4 = (CH2)2O(CH2)2, R5 = 4-ClC6H4] (II) was prepared by standard direct esterification of the corresponding acid (Z = OH) using H2SO4 catalyst in refluxing MeOH (75% yield). II was slightly more potent than carbamazepine in the maximal electroconvulsion test in mice, and had a significantly higher protective index against neurotoxicity (36 vs. 5.1). General synthetic methods, addnl. biol. results, and capsule formulations are described.

IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticonvulsant and analgesic)

RN 135548-47-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)

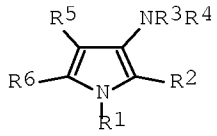


L3 ANSWER 38 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:469725 CAPLUS Full-text
DOCUMENT NUMBER: 117:69725
ORIGINAL REFERENCE NO.: 117:12263a,12266a
TITLE: Process for preparation of 2-substituted 3-aminopyrroles useful as anticonvulsives and analgesics
INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Ger. (East), 6 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298917	A5	19920319	DD 1989-340207	19891117
PRIORITY APPLN. INFO.:			DD 1989-340207	19891117

OTHER SOURCE(S): CASREACT 117:69725; MARPAT 117:69725
GI

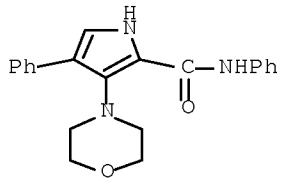


I

AB Nine title compds. I [R1 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl, acyl, alkoxycarbonyl, amino(thio)carbonyl; R2 = CHO, acyl, CO2H, alkoxycarbonyl, (un)substituted amino(thio)carbonyl, (hetero)aryl, NO2, cyano; R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl; R4 = (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl; or R3R4 = alkylene bridge optionally containing O, S, or N as ring atoms; R5 = (un)substituted (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene bridge] were prepared by reaction of 2-unsubstituted I (R2 = H) with corresponding electrophiles, e.g., acid chlorides, anhydrides, or isocyanates. For example, I [R1 = R6 = H, R2 = CO2Me, R3R4 = (CH2)2O(CH2)2, R5 = Ph] (II) was prepared in 56% yield by acylation of the corresponding I (R2 = H) with ClCO2Me in refluxing MeCN. At 10-3 mol/kg orally in mice in the hot-plate test, II gave 90% inhibition, vs. 55% for analgin. General prepns., addnl. biol. results, and capsule formulations are described.

IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticonvulsive and analgesic)

RN 135548-47-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



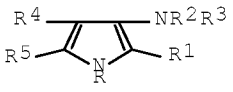
L3 ANSWER 39 OF 43 CAPLUS

ACCESSION NUMBER: 1991:492063 CAPLUS Full-text
DOCUMENT NUMBER: 115:92063
ORIGINAL REFERENCE NO.: 115:15835a,15838a
TITLE: Analgesic and anticonvulsant 3-aminopyrroles,
INVENTOR(S): Liebscher, Juergen; Knoll, Alexander; Uschmajew, Alexej; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter
PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 431371	A1	19910612	EP 1990-121958	19901116
EP 431371	B1	19970910		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
DD 298912	A5	19920319	DD 1989-334670	19891117
SI 20323	A	20010228	SI 1990-12173	19901115
FI 9005689	A	19910518	FI 1990-5689	19901116
FI 102169	B	19981030		
FI 102169	B1	19981030		
HU 56343	A2	19910828	HU 1990-7176	19901116
JP 03271271	A	19911203	JP 1990-311258	19901116
JP 07113015	B	19951206		
US 5502051	A	19960326	US 1990-614459	19901116
RU 2060991	C1	19960527	RU 1990-4831894	19901116
ES 2108005	T3	19971216	ES 1990-121958	19901116
RU 2120796	C1	19981027	RU 1994-2476	19901116
US 5684160	A	19971104	US 1995-446000	19950519

PRIORITY APPLN. INFO.: DD 1989-334670 A 19891117
YU 1990-2173 A 19901115
US 1990-614459 A3 19901116

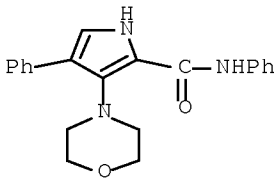
OTHER SOURCE(S): MARPAT 115:92063
GI



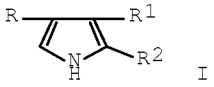
I

AB Aminopyrroles I [R = H, (un)substituted alkyl, cycloalkyl, aryl, heteroaryl, acyl, alkoxycarbonyl, carbamoyl, thiocarbamoyl; R1 = H, acyl, CO2H, alkoxycarbonyl, aryloxycarbonyl, carbamoyl, thiocarbamoyl, aryl, heteroaryl, cyano, NO2; R2, R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, aryl, heteroaryl; NR2R3 = heterocyclic; R4 = (un)substituted aryl, heteroaryl; R5 = H, alkyl, aryl, halogen; R4R5 = alkylene] were prepared by various methods. I (R = R5 = H, R1 = CO2Me, NR2R3 = morpholino, R4 = 4-ClC6H4), had an oral ED50 in the maximum electroshock test of 4.5 + 10-5 mg/kg. I (R = R5 = H, R1 = CO2H, CO2Me, NR2R3 = morpholino, R4 = Ph) caused 84.2 and 71.3% resp. inhibition of AcOH-induced writhing in mice.
IT 135548-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 135548-47-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)

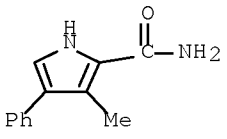


L3 ANSWER 40 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:55811 CAPLUS Full-text
DOCUMENT NUMBER: 108:55811
ORIGINAL REFERENCE NO.: 108:9313a,9316a
TITLE: A simple synthesis of pyrroles
AUTHOR(S): Cohnen, Erich; Dewald, Renate
CORPORATE SOURCE: Beiersdorf A.-G., Hamburg, D-2000/20, Fed. Rep. Ger.
SOURCE: Synthesis (1987), (6), 566-8
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:55811
GI

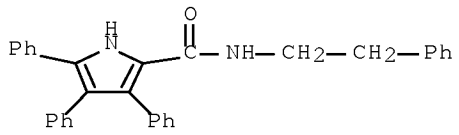


I

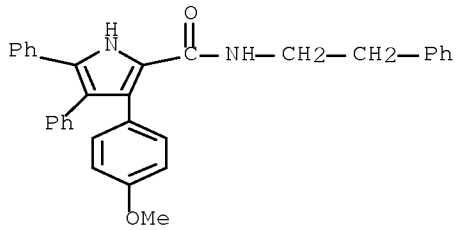
AB Cyclocondensation of Me2NCH:CRCOR1 (R = CO2Et, Ac, Bz, Ph, COCO2Et; R1 = Me, Et, Pr, Ph) with R3COCHR2NH2.HCl (R2 = CONH2, CN, Ac, CO2Et; R3 = NH2, Me) gave 35-97% 16 pyrroles I.
IT 112381-15-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
RN 112381-15-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-methyl-4-phenyl- (CA INDEX NAME)



L3 ANSWER 41 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:448869 CAPLUS Full-text
DOCUMENT NUMBER: 75:48869
ORIGINAL REFERENCE NO.: 75:7709a,7712a
TITLE: Independent syntheses of the products of acid- and base-catalyzed rearrangements of 2-(1-isoquinolyl)-3,3,5-triarylpyrrolenines
AUTHOR(S): McEwen, William E.; Berkebile, David H.; Liao, Tsung-Kai; Lin, Yun-Shan
CORPORATE SOURCE: Dep. Chem., Univ. Massachusetts, Amherst, MA, USA
SOURCE: Journal of Organic Chemistry (1971), 36(11), 1459-62
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2-(1-Isoquinolyl)-3,4,5-triphenylpyrrole (I) and 2-(1-isoquinolyl)-3-p-anisyl-4,5-diphenylpyrrole (II) were synthesized by unambiguous methods. The synthetic samples are identical with the products of the acid- or base-catalyzed isomerization of 2-(1-isoquinolyl)-3,3,5-triphenylpyrrolenine (III) and the base-catalyzed isomerization of 2-(1-isoquinolyl)-3-p-anisyl-3,5-diphenylpyrrolenine (IV), resp. By inference, 2-(1-isoquinolyl)-4-p-anisyl-3,5- diphenylpyrrole (V) is the product of the acid-catalyzed isomerization of IV.
IT 28506-38-9P 28638-50-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28506-38-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3,4,5-triphenyl-N-(2-phenylethyl)- (CA INDEX NAME)



RN 28638-50-8 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 3-(4-methoxyphenyl)-4,5-diphenyl-N-(2-phenylethyl)- (CA INDEX NAME)



L3 ANSWER 42 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:87561 CAPLUS Full-text
DOCUMENT NUMBER: 70:87561
ORIGINAL REFERENCE NO.: 70:16353a
TITLE: 4-Phenylpyrrole-2-carboxylic amides
INVENTOR(S): Hattori, Kiyoshi; Hashimoto, Masashi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 2 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

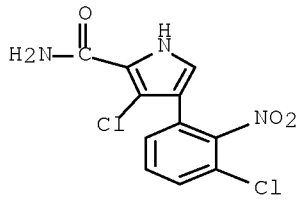
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 44001528	B4	19690123	JP	19660721

AB Manufacture of 3-chloro-4-(2-nitro-3-chlorophenyl)pyrrole-2-carboxamide (I), useful as a muscle relaxant, is described. Thus, 320 mg. 3-chloro-4-(2-nitro-3-chlorophenyl)pyrrole-2-carbonitrile is stirred with 7 cc. Me2CO, 250 mg. NaOH, and 3 cc. H2O, then stirred 30 min. more with 0.5 cc. 30% H2O2, let stand overnight with 1 cc. H2O, concentrated in vacuo, 10 cc. H2O added, and the precipitate recrystd. (AcOEt-C6H6) to give 76 mg. I, m. 202-3°.

IT 21765-13-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21765-13-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-chloro-4-(3-chloro-2-nitrophenyl)- (CA INDEX NAME)



L3 ANSWER 43 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:144086 CAPLUS Full-text
DOCUMENT NUMBER: 55:144086
ORIGINAL REFERENCE NO.: 55:27263f-i,27264a-i,27265a-i,27266a-e
TITLE: A new route to the synthesis of the pyrrole ring system
AUTHOR(S): Dimroth, Karl; Pintschovius, Ulrich
CORPORATE SOURCE: Univ. Marburg, Germany
SOURCE: Justus Liebigs Annalen der Chemie (1961), 639, 102-24
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:144086
GI For diagram(s), see printed CA Issue.

AB N-Alkyl, N-aryl, or N-acylamines, containing in α,α'-positions 2 CH2 groups activated by carbalkoxy or nitrile groups, condensed with Bz2 in the presence of Me3COK in 60-80% yields to 1-alkyl(aryl or acyl)-3,4-diphenylpyrrole derivs. bearing in the 2- and 5-positions CO2H, carbalkoxy, CN, or carboxamide groups. The free pyrrole-α-carboxylic acids were readily decarboxylated by acids to the α,α'-unsubstituted pyrroles. The 1-acylpyrroles were hydrolyzed by bases to the pyrroles. The preparation of suitable CH2-containing amine components was described. A simple cyanomethylation procedure with polyoxymethylene (I), KCN, and AcOH was described for the conversion of aromatic amines to the previously unknown bis(cyanomethyl) derivs. Crude PhN(CH2CO2H)2 (55 g.), 250 cc. MeOH, and 20 cc. concentrated H2SO4 refluxed 7 hrs., concentrated in vacuo, diluted with iced H2O, and extracted with Et2O gave 73% PhN(CH2CO2Me)2 (II), b10 183°, m. 47-9°. Similarly prepared was PhN(CH2CO2Et)2, b10 188°. p-MeOC6H4NH2, 1 mole ClCH2CO2H, and 1.5 moles NaOAc.3H2O were converted to p-MeOC6H4NHCH2CO2H, which, heated 5 hrs. with 2.5 moles ClCH2CO2Na on the steam bath and then esterified in the usual manner with MeOH-H2SO4, gave p-MeOC6H4N(CH2CO2Me)2 (III), b11 209°; III.HCl, m. 136-7° (absolute MeOH). p-MeC6H4NH2 was converted similarly to p-MeC6H4N(CH2CO2Me)2 (IV), b10 186°, m. 44.5-45°. p-ClC6H4NHCH2CO2H (40 g.) in dilute aqueous solution of 8.7 g. NaOH treated below 35° with a solution of 70 g. Cl-CH2CO2H and 30 g. NaOH (total volume of mixture about 500 cc.), heated 4-5 hrs. on the water bath, cooled, and filtered, and the residue treated with 80 cc. 6N HCl gave p-ClC6H4N(CH2CO2Me)2 (V), b10 202-3°, m. 58-9°. p-H2NC6H4CO2H (13.7 g.) and 4 g. NaOH in H2O treated with aqueous ClCH2CO2Na from 28.5 g. ClCH2CO2H, heated 8 hrs. on the water bath, cooled, and filtered, and the residue treated with HCl gave 54% p-HO2CC6H4N(CH2CO2H)2 (VI), decomposing 260°. VI (15 g.), 50 cc. MeOH, and 6 cc. H2SO4 heated 7 hrs. on the water bath gave 14.8 g. p-MeO2CC6H4N(CH2CO2Me)2 (VII), m. 91-2° (EtOH or ligroine); VII.HCl decomposing 85-90°. II in CCl4 or AcOH treated with the calculated amount of Br at room temperature gave p-BrC6H4N(CH2CO2-Me)2 (VII), m. 64-6°, b10 216°; VII. H Br decomposing 130-1° (MeCN or EtCOMe). II (10 g.) in 100 cc. AcOH treated with stirring and cooling with 3.3 cc. colorless 100% HNO3 and poured after a few min. onto ice yielded 75-80% (crude) p-O2NC6H4N(CH2CO2Me)2 (VIII), yellow-brown needles with a bluish luster, m. 123-3.5° (CCl4 or MeOH). Similarly prepared was p-O2NC6H4N(CH2CO2Et)2 (IX), 87%. m. 137°, which (hydrolyzed with alkali) gave p-O2NC6H4N(CH2CO2H)2, decomposing 202-5°. VIII reduced with Na2S2O4 in aqueous EtOH and extracted with CHCl3 gave p-H2NC6H4N(CH2CO2Me)2, m. 53-5°, b0.01 156-9°; HCl salt decomposing 205-6°. NaHSO3 (208 g.) in a min. of H2O treated with 150 cc. 40% aqueous CH2O, the mixture treated after 20 min. with stirring with 100 g. 30% aqueous MeNH2, heated 20 min. on the water bath, treated with 134 g. KCN in 250 cc. H2O, saturated with NaCl, and extracted with Et2O yielded 48% MeN(CH2CN)2 (X), b11 130°; X.HCl decomposing 120-2°. p-O2NC6H4NMe2 (33 g.), 18.7 cc. 38% CH2O, and 26 g. NaHSO3 heated 15 min. at 100° with occasional shaking and treated with 16.5 g. KCN in 30 cc. H2O yielded 31.5 g. crude p-Me2NC6H4N(CH2CN)Me (XI), m. 80°. Powdered KCN (8 g.), 14 g. XI, and 2.8 g. I treated with cooling with 65 cc. AcOH, heated 1 hr. at 50°, stirred several hrs., and poured into iced H2O gave 13.6 g. p-Me2NC6H4N(CH2CN)2 (XII), m. 127-8.5° (BuOH-EtOH); XII.HCl decomposing 207-10° (85% EtOH). NaHSO3 (35 g.) and 25 cc. 38% aqueous CH2O treated on the water bath with 41 g. p-MeOC6H4NH2 and then with 22 g. KCN in 50 cc. H2O and heated 20 min. on the water bath gave 42 g. p-MeOC6H4NHCH2CN (XIII), m. 75-6° (MeOH or CCl4). XIII (15.2 g.), 8.5 g. KCN, and 3.8 g. I treated dropwise with stirring and cooling with 100 cc. AcOH containing 3 drops concentrated H2SO4, heated 4 hrs. at 40-50°, and kept overnight yielded 18.3 g. p-MeOC6H4N(CH2CN)2 (XIV), m. 114-15°, b9 221.5°. PhNHCH2CN (26.4 g.), b11 63°, with 17 g. KCN, 7.6 g. I, and 150 cc. AcOH gave 80% (crude) PhN(CH2CN)2 (XV), leaflets, m. 139-40° (BuOH). II with absolute EtOH and NH3 gave PhN(CH2CONH2)2 (XVI). XVI (10 g.) in 25 cc. Decalin heated 0.5 hr. at 180° with 10 g. P2O5 and extracted with C6H6 gave some XV; the mother liquor

yielded 4-phenyl-2.6-piperazinedione. m. 159-60°. p-MeC6H4NHCH2CN (20.5 g.), 11.5 g. KCN, 5.3 g. I. and 100 cc. AcOH gave 88% p-MeC6H4N(CH2CN)2, m. 119-20° (MeOH), b11 207°. p-MeC6H4NHCH2CO2Me (27 g.) (from 10 g. p-MeC6H4NH2 and 5.1 g. ClCH2CO2Me), m. 84-6°, 12.5 g. KCN, 6 g. I, and 100 cc. AcOH kept at 35° and then heated 2 hrs. at 50° gave 32.1 g. p-MeC6H4N-(CH2CN)CH2CO2Me (XVII), b10 195-5.5°, m. 80-1°. p-MeC6H4NHCH2Bz (14 g.) with 5 g. KCN, 2.3 g. I, and 60 cc. AcOH yielded (at 40°) p-MeC6H4N(CH2CN)CH2Bz, greenish crystals, m. 153-4.5°. PhNH2 (9.3 g.) and 35.2 g. iso-Pr2NEt treated at 0° with stirring with 40 g. BzCH2Br in 40 cc. CHCl3 and the mixture refluxed 0.5 hr., cooled, and filtered yielded 17.7 g. PhN(CH2Bz)2 (XVIII), m. 225-8° (MeOCH2CH2OH). BzCH2NHPh (26 g.) with 28.2 g. BzCH2Br and 17 g. iso-Pr2NEt refluxed in 40 cc. CHCl3 gave XVIII. III (2.7 g.) and 1.5 g. (CO2Et)2 (XIX) treated with 0.9 g. Na in 20 cc. MeOH, kept several days, warmed, and filtered, and the residue treated with HCl gave 1-(p-methoxyphenyl)-3,4-dihydroxypyrrole-2,5-dicarboxylic acid di-Me ester (XX), m. 185-8° (with gas evolution) (MeOCH2-CH2OH and EtCOMe). IX (4.0 g.) and 2.2 g. XIX in 60 cc. Me3COH treated at 50° with 1.2 g. K in 40 cc. Me3COH, kept 15 hrs., and evapd, in vacuo, and the residue extracted with MeOH gave 1-(p-nitrophenyl)-3,4-dihydropyrrole-2,5-dicarboxylic acid di-tert-Bu ester, m. 176-8° (AcOH, EtOH, and ligroine); it gave a green FeCl3 reaction. BzH (5 cc.) and 5 g. II in 20 cc. MeOH added dropwise at 2-5° to 2 g. Na in 30 cc. absolute MeOH, kept 2 hrs. at 0°, evaporated in vacuo below 30°, treated with cold HCl, and extracted with MeOH yielded 1.5 g. PhN[C(:CHPh)CO2H]2, greenish yellow crystals, m. 161-3°; the mother liquor gave PhCH:C.NPh.CH2.CHPh.O.CO, m. 223-5° (decomposition) (85% AcOH); the filtrate diluted with CH2Cl2 precipitated a Na salt, which (triturated with concentrated HCl) gave BzCO2H, m. 14750°; it gave a dark green FeCl3 reaction. The filtrate from the BzCO2H treated with Br gave 2,4-Br2C6H3NHCH2CO2H, prisms, m. 161° (petr. ether). Bz2 (5.3 g.) and 6.0 g. II in 30 cc. dry Et2O added dropwise with cooling and stirring to 4 g. K in 60 cc. absolute Me3COH and 20 cc. dry Et2O, the mixture kept 20 hrs. and evaporated below 40° in vacuo, and the residue treated with a small amount of H2O gave 1.3 g. yellow K salt (yellow in concentrated H2SO4), which (recrystd. from AcOH with heating) gave 1,3,4-triphenylpyrrole, needles, m. 150-7°, intense orange in concentrated H3SO4; it coupled with diazonium salts in AcOH. III (10 g.), 7.0 g. Bz2 in 50 cc. Et2O, and 5 g. K in 90 cc. Me3COH gave (in the usual manner during 20 min.) the 2-CO2Me derivative (XXI) of 1-(p-methoxyphenyl)-3,4-diphenylpyrrole (XXII), m. 169.5-71° (iso-AmOAc), and from the mother liquor the 2-CO2CMe3 derivative (XXIII) of XXII, needles, m. 128-9° (absolute EtOH). XXI refluxed 4 hrs. with 10% alc. KOH gave the carboxylic acid, m. about 200°, which (heated with a little H2SO4) gave XXII, prisms, m. 109-10° (EtOH). XXIII refluxed 5 hrs. with 5 drops concentrated HCl in 25 cc. EtOH gave also XII. IV (6.0 g.), 5.0 g. Bz2, and 4 g. K in 90 cc. Me3COH and 20 cc. Et2O neutralized after 4 hrs. with HCl, filtered, and evaporated gave 6 g. (crude) 1-(p-MeC6H4) analog (XXIV) of XXI, prisms, m. 130.5-31° (5:1 MeOH-C6H6). XXIV refluxed 4 hrs. with alc. KOH and decarboxylated with concentrated H2SO4 yielded the 2-CO2H derivative (XXV) of 1-(p-MeC6H4) analog (XXV) of XXII, m. 179-82°, which, recrystd. from AcOH and ligroine, yielded XXV, leaflets, m. 130-1° (AcOH-ligroine). Bz2 (5 g.) and 6.7 g. V condensed in the usual manner, treated after 4 hrs. with 10 cc. concentrated HCl, filtered, and kept some time at room temperature deposited 2.3 g. 1-(p-ClC6H4) analog (XXVI) of XX, m. 204.5-205°, with gas evolution (BuOH-EtOH and MeNO2), yellow in concentrated H2SO4; the mother liquor evaporated gave the p-ClC6H4 analog (XXVII) of XXI, prisms, m. 118-20° (EtOH and AcOH). XXVI and XXVII saponified with alkali and decarboxylated gave the 1-(p-ClC6H4) analog of XXII, m. 145-6° (AcOH or EtOH). K (3.8 g.) in 70 cc. Me3COH, 4.6 g. Bz2 in 20 cc. Et2O, and 7.6 g. VII in 30 cc. Me3COH heated 3 hrs., neutralized with HCl, and filtered, and the filtrate concentrated gave 3.0 g. (crude) 1-(p-BrC6H4) analog (XXVIII) of XX, prisms, m. 190-1° (3:1 BuOH-EtOH). XXVIII saponified with alkali and heated with H2SO4 gave the 1-(p-BrC6H4) analog of XXII, m. 135-7° (ligroine and AcOH). VI (5.5 g.) and 4.5 g. Bz2 in 160 cc. Et2O

treated 20 min. at 5° with 7.4 g. K in 85 cc. Me3COH, the mixture evaporated in vacuo, adjusted with HCl to pH 8, and filtered, and the resinous residue (10 g.) refluxed 2 hrs. with alc. KOH, acidified, and ground with AcOH gave 1.6 g. 1-(p-HO2CC6H4) analog of XXII, m. 241-3°, with browning (AcOH and AmOAc), yellow in concentrated H2SO4. VIII (7 g.), 5 g. Bz2, and 3.8 g. K in 65 cc. Me3COH, 90 cc. Et2O, and 70 cc. dioxane kept 1 hr. at 5°, treated with 5 cc. AcOH, and evaporated, the residue washed with H2O and dissolved in CHCl3, and the CHCl3 solution washed with aqueous NaHCO3 (to remove about 0.6 g. organic acid) and evaporated gave a substance, m. 211-13° (light red in concentrated H2SO4), which could not be eluted from Al2O3 when chromatographed; the mother liquor chromatographed twice on Al2O3 gave the 1-(p-O2NC6H4) analog (XXIX) of XXI, m. 193-5° (EtCOMe, AcOH, BuOH), intense orange-yellow in concentrated H2SO4; it gave a red dye with diazonium salts. K (3.4 g.) in 70 cc. Me3COH, 5 g. XIV, and 5 g. Bz2 in dioxane-Me3COH treated with AcOH, evaporated in vacuo, and extracted with H2O left 9.8 g. 1-(p-methoxyphenyl)3,4-diphenyl-2-cyanopyrrole-5-carboxamide (XXX), prisms, m. 248.5-49° (BuOH). XVII (5.5 g.), 3.5 g. K in 100 cc. Me3COH, and 5.3 g. Bz2 in 50 cc. Me3COH and 7 cc. dioxane treated with AcOH yielded similarly 8.2 g. 2-CN derivative of XXV, m. 142-2.7° (AcOH and ligroine). XII (4.3 g.) condensed during 2 hrs. with 4.2 g. Bz2 and 3.4 g. K in 50 cc. Me3COH and 50 cc. dioxane and evaporated, and the residue ground with warm MeOH and diluted with C6H6 precipitated the 1-(p-Me2NC6H4) analog (XXXI) of XXX, m. 283°, with browning at 270° (HCONH2); the mother liquor gave 1-(p-dimethylaminophenyl)-3,4-dihydroxy-3,4-diphenyl- 2,5-dicyanopyrrolidine (XXXII), m. 221-3° (decomposition), which (triturated with 33% HCl) gave XXXII.HCl. K (4 g.) in 65 cc. Me3COH condensed at 0° with 3.3 g. X and 6.3 g. Bz2 in 75 cc. Et2O, the mixture kept overnight and filtered, and the residue triturated with 80% AcOH gave 6 g. 1-Me analog of XXX, m. 276° colorless in concentrated H2SO4; the mother liquor gave a small amount of 1-methyl-3,4-diphenyl-2,5-dicyanopyrrole, m. 159-61° (90% EtOH). K (4 g.) in 85 cc. Me3COH and 10 cc. Et2O condensed with 5.25 g. Bz2 and 7 g. AcN(CH2CO2Me)2, m. 83.5-84°, b15 184°, in 40 cc. Me3COH and 15 cc. dioxane, the mixture evaporated, washed with Et2O, dissolved in H2O, and acidified with HCl gave 1-acetyl-3,4-diphenylpyrrole-2,5-dicarboxylic acid (XXXIII), m. 254-5° (decomposition) (aqueous MeOH); the Et2O-insol. residue chromatographed gave the Me ester (XXXIV) of XXXIII, m. 143-4° (MeOH). The residue from the Et2O washing (4.6 g.) ground with MeOH and recrystd. repeatedly from PhMe-ligroine gave 3,4-diphenylpyrrole-2-carboxylic acid tert-Bu ester, leaflets, m. 164-5°, yellow in H2SO4. XXXIV refluxed 3 hrs. with 1.3 g. KOH in 20 cc. EtOH gave 3,4-diphenylpyrrole-2-carboxylic acid, m. 205-7°. BzN(CH2CN)2 (4 g.), m. 131-2°, and 4.1 g. Bz2 in 40 cc. dry tetrahydrofuran and 35 cc. dry MeCN treated 1.5 hrs. with 1.6 g. K in 40 cc. Me3COH and 50 cc. dry C6H6, stirred 3.5 hrs. at 20°, treated with 3.4 g. AcOH, filtered, and concentrated in vacuo to 1/3 volume yielded 1.3 g. 1-Bz analog (XXXV) of XXX, m. 239-41° (decomposition) (EtOH and iso-PrOH); the concentrated filtrate from the crude product diluted with Et2O gave 3,4-diphenyl-2-cyanopyrrole-5-carboxamide (XXXVI), m. 294-7° (decomposition) (iso-Am2O and MeOH). XXXV refluxed 8 hrs. with 4% alc. KOH gave 1.15 g. XXXVI, needles, m. 299-300° (MeCN-iso-PrOH). K (6.3 g.) in 100 cc. Me3COH added to 9 g. acenaphthenequinone and 10 g. II in 50 cc. dry C6H6, refluxed 0.5 hr. and evaporated in vacuo, the residue extracted with Na2CO3, and the extract acidified carefully precipitated a mono-Na salt, which (with HCl) yielded 1.2 g. 1-phenyl-3,4-dihydroxy-3,4-(1,8- naphthylene)pyrrolidine-2,5-dicarboxylic acid, decomposing 221-2° (AcOH and 1:1 aqueous Me2CO). XXXII (7 g.) in 100 cc. dry dioxane with 4.5 g. Bz2 and 2.2 g. K in 40 cc. Me3COH heated 5 hrs. at 35°, adjusted with HCl to pH 5, and filtered, and the filtrate evaporated gave about 1 g. 1-phenyl-2,5-dibenzoyl-3,4-dihydroxy-3,4-diphenylpyrrolidine, yellowish needles, decomposing 221-4° (Et2CO), pale red in warm concentrated H2SO4. The infrared absorption spectra of XII, XXXI, and XXXII were recorded.

IT 101605-72-5P, Pyrrole-2-carboxamide, 5-cyano-3,4-diphenyl-
101895-84-5P, Pyrrole-2-carboxamide,

5-cyano-1-methyl-3,4-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 101605-72-5 CAPLUS
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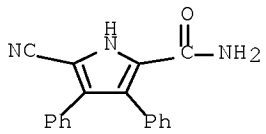

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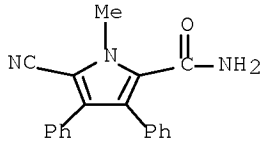

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